Report No. A049-2
September 1989

Prepared for
State of California
Air Resources Board
Sacramento, California 95812

Prepared Under
Contract No. A6-215-74

CALGRID: A Mesoscale Photochemical Grid Model
Volume II: User's Guide

Prepared by
J.S. Scire, Sigma Research Corporation
R.J. Yamartino, Sigma Research Corporation
G.R. Carmichael, University of Iowa
Y.S. Chang, University of Iowa

Contents

1 Introduction

1.1 Background

In July, 1987, the California Air Resources Board (ARB) initiated a project to upgrade and modernize the Urban Airshed Model (UAM) It was specified that the new model contain state-of-the-science improvements in many of the key technical algorithms, including the horizontal and vertical transport and diffusion schemes. the dry deposition model, the chemical mechanism, and the chemical integration solver. In addition, it was required that the model be coded as structured ANSI 77 FORTRAN, contain extensive internal documentation, and include a dynamic memory allocation scheme to facilitate efficient computer usage over a wide range of potential applications.

Our first task was to dissect the existing UAM to determine those portions that needed to be replaced. When the UAM was developed over a decade ago, computers and computer languages were very different than they are today. Computers, for example, tended to have small amounts of core storage memory. As a result or this, UAM developers adopted innovative methods to save memory, such as having the option to split up the grid, which created the need for additional intermediate data files and input/output (I/O) overhead. In addition the FORTRAN language had not yet experienced the beneficial impacts of structured programming concepts The UAM code also clearly reflected years of modification and correction by a number of programmers and scientists. Thus, after several months of effort we made the difficult decision to start over "from scratch" and build a new model. As we were simultaneously constructing a new non-steady-state dispersion model (`CALPUFF`) and associated meteorological driver package (`CALMET`), it was decided that the new photochemical model should be driven by (or drivable by) `CALMET`. Thus, the resultant model has been given the new name `CALGRID`, both to indicate that it is no longer "just" an updated UAM, but also to suggest that it can be run "in parallel" with the `CALPUFF` model.

The above mentioned PUFF/GRID parallel aspect is an important complementary feature in complete impact assessments because `CALPUFF` excels at estimating primary pollutant concentrations and source culpabilities in the absence of highly non-linear chemistry effects, whereas `CALGRID` is most reasonable for secondary pollutant species, such as ozone, arising out of highly non-linear chemistry. Such dual modeling approaches are likely to play a greater role in management planning and emissions reduction scenario evaluation as the country moves fully into the post '87 oxidant control strategy milieu.

1.2 Overview of the Modeling System

The overall modeling system configuration showing the CALMET, CALGRID, and postprocessing components is presented in Figure 1.2-1. The major components of the modeling system are summarized below.

CALMET is a meteorological model which includes overland and overwater boundary layer modules and a diagnostic wind field generator. The overwater boundary layer formulation uses actual or climatological overwater meteorological data to predict the turbulence parameters in the marine boundary layer. An energy balance method is used to describe heat fluxes and turbulence parameters over land. The diagnostic wind field module contains parameterized treatments of slope flows, kinematic terrain effects, terrain blocking effects, and a divergence minimization procedure.

CSUMM (a version of the Colorado State University Mesoscale Model) is a primitive equation wind field model for the simulation of mesoscale airflow resulting from differential surface heating and terrain effects. The prognostic CSUMM model Is well-suited for simulation of sea-breeze circulations, heat island effects, and mountain-valley circulations. CALMET contains options to allow wind fields produced by CSUMM to be combined with observational data and/or interpolated to finer grid scales.

CALGRID is an Eulerian photochemical transport and dispersion model, which includes modules for horizontal and vertical advection/diffusion, dry deposition, and one of the State Air Pollution Research Center (SAPRC) family of photochemical mechanisms.

POSTPRO is a postprocessing program with options for the computation and display of time-averaged concentrations and dry deposition fluxes produced by the CALGRID model.

PRTMET is a postprocessor which allows user-selected fields of winds and/or micrometeorological variables to be extracted from the CALMET.DAT data file and displayed.

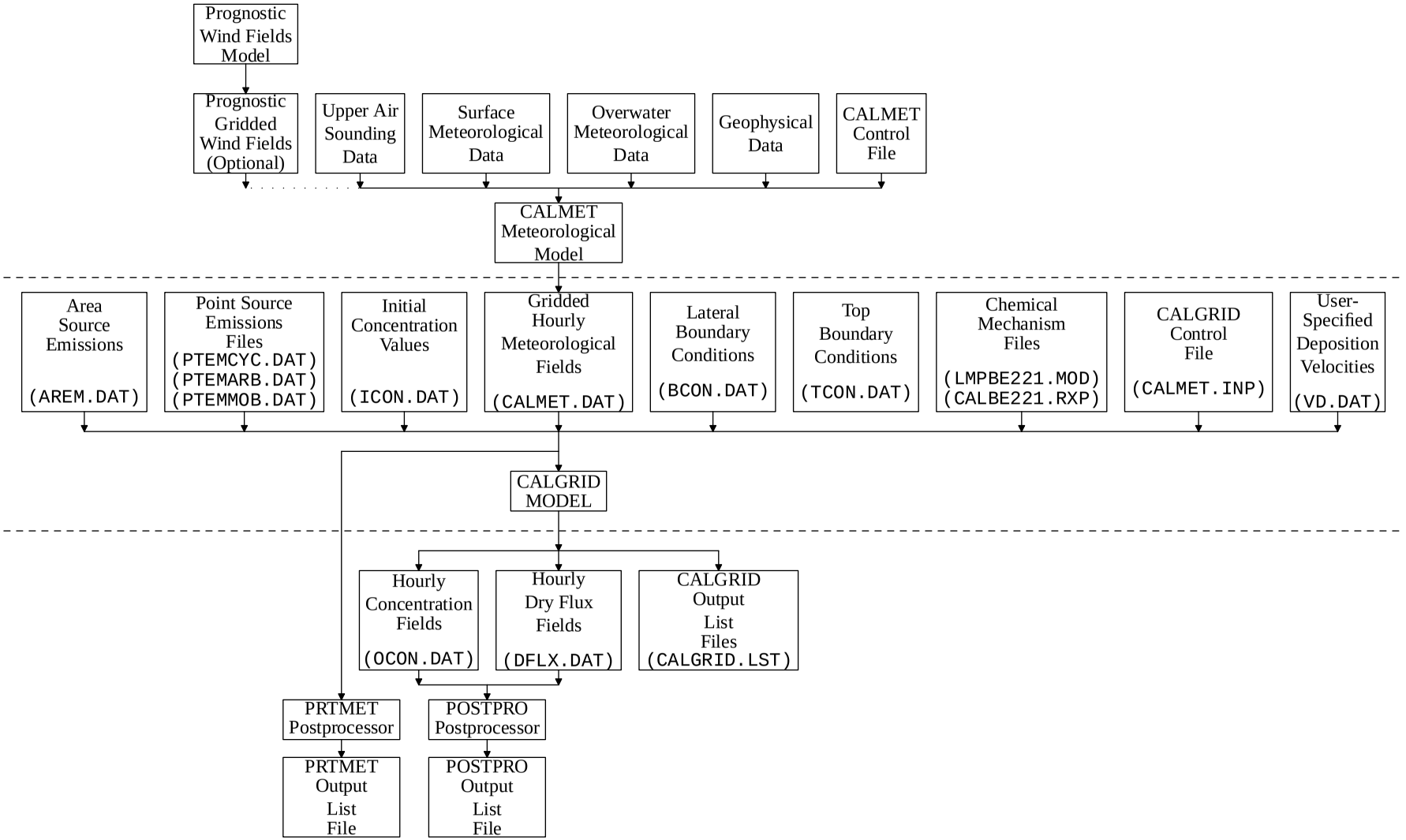

Figure 1.2-1: CALGRID Modeling System Flow Diagram

The Model Formulation Document and User's Guide for the CALPUFF modeling system (Scire et al., 1989 a,b) describe the CALMET meteorological model and the postprocessing programs (as well as the CALPUFF model) in detail. Douglas and Kessler (1989) and Kessler (1989) describe the diagnostic and prognostic wind field components of the modeling system in more detail. Additional information regarding CALGRID can be found in the companion Model Formulation Document (Yamartino et al., 1989).

1.3 Major Model Features and Options

The major technical components upgraded as part of the CALGRID development project include the following:

Chemical Mechanism and Solver: The currently implemented mechanism is a version of the Carter, Atkinson, Lurmann, Lloyd (CALL) scheme developed for the ARB under a separate contract. to the State Air Pollution Research Center (SAPRC). This family of schemes is now referred to as the SAPRC mechanisms. The current version of CALGRID uses the SAPRC mechanism known as LMPBE221. This mechanism involves 2 alkanes, 2 aromatics, and 2 alkenes, 19 directly emitted species, 36 advected (27 active plus 9 buildup) plus 10 steady state chemical species, and 102 chemical reactions. CALGRID uses procedures developed by Carter (1988) for the computerized generation of the chemical mechanism. These procedures allow the chemical mechanism to be easily modified or exchanged without requiring extensive recoding of the model.

A chemical integration solver is based on the quasi-steady-state method (QSSA) of Hesstvedt et al. (1978) and Lamb (1984). This solver can efficiently and accurately handle the stiffest of modern schemes.

Vertical Transport and Diffusion: A vertical transport and diffusion scheme is provided that incorporates the latest boundary formulations, permits arbitrary and spatially varying spacing of vertical levels, and accounts for all vertical flux components of moving or stationary levels. The vertical diffusivities in CALGRID are based on convective scaling in the daytime boundary layer and local or z-less scaling in the nighttime boundary layer.

Horizontal Transport and Diffusion: A high-order chapeau function scheme is implemented in CALGRID for solving the horizontal advective/diffusion equation. This scheme conserves mass exactly, prohibits negative concentrations, and exhibits very little numerical diffusion. Several options are provided for the computation of horizontal diffusivities, including the Smagorinsky (1963) method, or user-specified stability-dependent values.

Dry Deposition: A full resistance-based model is provided in CALGRID for the computation of dry deposition rates of gases and particulate matter as a function of geophysical parameters, meteorological conditions, and pollutant species. An option is provided to allow user-specified, diurnally varying deposition velocities to be used for one or more pollutants instead of the resistance model (e.g., for sensitivity analyses).

1.4 Summary of Data and Computer Requirements

Data Requirements

The input data sets used by CALGRID are summarized in Table 1.4-1 (also see the modeling system flow diagram, Figure 1.2-1). CALGRID reads user inputs from a "control file" called CALMET.INP. This file contains the user's selection for the various model options, technical input variables, output options, etc. A meteorological data file (CALMET.DAT) contains hourly gridded fields of micrometeorological parameters and three-dimension wind and temperature fields. The meteorological data file also contains geophysical data such as terrain heights which are required both by the meteorological model (e.g., for terrain adjustment of the wind fields) and by the CALGRID model. The required contents of the CALMET.DAT input file and the other input data bases are summarized in Table 1.4-2.

Table 1.4-1
Summary of CALGRID Input Files

FILE NAME	CONTENTS	UNIT* NUM.	TYPE
CALGRID.INP	Control file inputs	IO5	Formatted
CALMET.DAT	Geophysical and hourly meteorological data	IO7	Unformatted
ICON.DAT	Initial concentrations	IO10	Formatted or Unformatted
BCON.DAT	Lateral boundary conditions (Optional)	IO11	Formatted or Unformatted
TCON.DAT	Top boundary conditions (Optional)	IO12	Formatted or Unformatted
PTEMCYC.DAT	Emission data for point sources with cyclical or constant emission parameters (Optional)	IO15	Unformatted, Direct-Access
PTEMARB.DAT	Emission data for point sources with arbitrarily-varying emission parameters (Optional)	IO16	Unformatted
PTEMMOB.DAT	Emission data for mobile point sources (Optional)	IO17	Unformatted
AREM.DAT	Emissions data for area sources (Optional)	IO18	Unformatted
VD.DAT	User-specified deposition velocities (Optional)	IO20	Formatted
LMPBE221.MOD	Chemical mechanism definition file	31	Formatted
CALBE221.RXP	Emission-specific chemical data file	32	Formatted

* Variable shown is the parameter controlling the FORTRAN unit number associated with the file. Usually, the value associated with the parameter is consistent with the name (i.e., IO10 = 10). However, the value can be easily changed in the parameter file to accommodate reserved unit numbers on a particular system.

Table 1.4-2
Summary of Input Data Required by CALGRID

Geophysical Data (CALMET.DAT**)**

Gridded fields of:

- surface roughness length (z_0)
- land use categories
- terrain elevations
- leaf area index

Meteorological Data (CALMET.DAT**)**

Gridded fields of:

- u, v, W wind components (3-D)
- air temperature (3-D)
- surface friction velocity (u_*)
- mixing height (z_i)
- convective velocity scale (w_*)
- Monin-Obukhov length (L)
- PGT stability class

Hourly values of the following at the surface met stations:

- air density (ρ_a)
- air temperature
- short-wave solar radiation
- relative humidity

Emission Data

Point Source Emissions:

- constant or cyclical emission parameters (PTEMCYC.DAT)
- arbitrarily-varying emission parameters (PTEMARB.DAT)
- mobile point sources (PTEMMOB.DAT)

Area Source Emissions:

- gridded fields for each emitted species (AREM.DAT)

Initial and Boundary Conditions

Initial Concentrations (ICON.DAT):

- formatted file with one value per layer per species, or
- unformatted file with a full 3-D set of initial concentrations

Lateral Boundary Conditions (BCON.DAT):

- formatted file With user-defined boundary types and time-independent values as a function of height for each species, or
- unformatted file with a complete set of time-dependent boundary conditions for each species

Top Boundary Conditions (`TCON.DAT`):

- formatted file with one time-independent value for each species, or
- unformatted file with a full 2-D field of time-dependent values for each species

Chemistry Data

- chemical mechanism definition file (`LMPBE22l.MOD`)
- emissions-specific chemical data (`CALBE22l.RXP`)

Deposition Velocity Data

- One deposition velocity for each user-specified species for each hour of a diurnal cycle

Three types of files are provided for point source emissions: stationary sources with constant or cyclical emissions, (e.g., daily or weekly cycles), stationary sources with arbitrarily varying emissions, and mobile point sources (e.g., ships). A gridded area source inventory is also allowed in CALGRID. Ordinary motor vehicle emissions are contained in the area source file.

Additional files contain the starting concentrations for the model, concentrations at the lateral boundaries of the model domain, and concentrations above the top of the model's highest layer.

The model also requires two chemical data files: one which defines chemical mechanisms and a second which contains emissions-specific chemical parameters. These files are designed to be directly compatible with the chemical and emissions processing system developed by Carter (1988).

An additional file containing diurnal cycles of user-specified deposition velocities is required if the user requests that input deposition velocities be used instead of the resistance model for any of the deposited pollutants.

As indicated in Table 1.4-2, CALGRID provides options for different levels of detail in several of the data sets, such as the initial concentrations, lateral boundary conditions, and top boundary conditions. For example, these files may be formatted files with limited space-time variations to the data, or more complete unformatted files with full space and time variability. The emissions data files are organized to reduce disk storage requirements and maintain an optimal structure for each type of emissions source: point sources with constant or cyclical emissions, arbitrarily varying emissions, mobile sources, and area sources.

The options available for each data set and its structure, format, and contents are described in detail in Chapter 4.

The CALGRID output files are summarized in Table 1.4-3. The list file contains a copy of the inputs used in the run, a summary of the memory requirements of the run, optional (user-selected) gridded fields of the predicted one-hour averaged concentrations, dry fluxes, top fluxes, deposition velocities, total emissions (point and area sources), as well as any messages generated during the simulation. The CONC.DAT and DFLX.DAT files contain the output concentrations and dry fluxes in an unformatted form suitable for further processing by the postprocessing program, POSTPRO. A fourth output file, CHMOUT1, summarized the setup of the chemical mechanism for the current run.

Computer Requirements

Table 1.4-3
Summary of CALGRID Output Files

FILE NAME	CONTENTS	UNIT* NUM.	TYPE
CALGRID.LST	List file produced by CALGRID	IO6	Formatted
CONC.DAT	Gridded fields of one-hour averaged concentrations (ppm) for species and levels selected by the user in the control file	IO8	Unformatted
DFLX.DAT	Gridded fields of one-hour averaged dry deposition fluxes ($g/m^2/s$) for species selected by the user in the control file	IO9	Unformatted
CHMOUT1	List file produced by the initialization phase of the chemistry module	33	Formatted

* Variable shown is the parameter controlling the FORTRAN unit number associated with the file. Usually, the value associated with the parameter is consistent with the name (i.e., IO10 = 10). However, the value can be easily changed in the parameter file to accomodate reserved unit numbers on a particular system.

Table 1.4-4

CPU Requirement (% of TOTAL CPU Runtime) of CALGRID by Module Based on a 12-Hour Test Run with a 20 by 20 Horizontal Grid, 10 Vertical Layers, Time Step of 1200 Seconds, and the LMPBE221 Chemical Mechanism Solved Using the QSSA Method.

Horizontal Advection/Diffusion	20.5%
Vertical Advection/Diffusion, Emissions injections, Dry Deposition	7.4%
Chemistry	71.4%
Miscellaneous Other Computational Routines	0.6%
Setup, Termination Phases	0.5%
Total	100.0%

The memory management system used in CALGRID is designed to allow the array parameters to be easily adjusted to match the requirements of a particular run either through internal allocation of subarrays via the use of a master array or by modifying parameter statements in a parameter file controlling array dimensions.

Therefore, the memory required by CALGRID will be determined by the particular application. However, as an example, CALGRID required approximately 2 Mbytes of memory for a test application with a 20 by 20 horizontal grid, 10 vertical layers, and 36 advected species.

This test run of CALGRID required approximately 0.45 seconds of CPU time per grid cell per time step on a 20 MHz SUN 3/60 workstation having a computational speed of about 0.15 MFlop. In the test run, the basic time step was 1200 seconds. Table 1.4-4 gives a breakdown of the CPU requirements of the various modules.

Over 70% of the CPU time was used in the solution of the chemical equations. The horizontal advection/diffusion module required nearly 21%, and vertical advection/diffusion, plume rise, and dry deposition together account for about 7% of the CPU required. The remaining 1% of the time was used in the setup or termination phase of the model or other miscellaneous computational routines.

2 Technical Description

2.1 Grid Systems

Horizontal Grid System

The CALGRID model uses a system of NX by NY square grid cells, as shown in Figure 2.1-1. The "grid point" refers to the center of each grid cell in both the horizontal and vertical dimensions. The horizontal computational grid must correspond to that used in the meteorological modeling in terms of the number of cells in the x and y directions, cell size, and reference origin coordinates.

The outer strip of grid cells are used as "boundary cells." Integration of the physical and chemical processes conducted in the model (e.g., advection, diffusion, dry deposition, emissions injection, and chemical transformation) is not performed for the boundary cells. These cells serve as storage locations for the lateral boundary concentrations of the grid. Therefore, the active region on the grid consists of (NX-2, NY-2) cells starting at grid cell (2,2) to (NX-1, NY-1).

The position of the computational grid system in real space is determined by the reference coordinates (XORIGKM, YORIGKM) of the southwest corner of grid cell (1,1). Thus, grid point (1,1) is located at (XORIGKM + DGRIDKM/2., YORIGKM + DGRIDKM/2.), where DGRIDKM is the length of one side of the grid square.

It is assumed that the orientation of the X and Y axes of the CALGRID computation grid are east-west and north-south, respectively. In this way, the grid system is directly compatible with the meteorological driver, CALMET, which produces u, v, wind fields components also defined with respect to east-west and north-south.

Vertical Grid System

Three options are provided for the vertical grid system in CALGRID. In all of these options, the coordinates are terrain following, with the top of the modeling domain a fixed height above the local terrain.

Option A: All layers below the mixing height except Layer 1 are of a uniform depth. Layer 1 is a fixed 20 m in depth. The layers above the mixing height are all of a second uniform depth. These layers can vary in both space and time, reflecting variation in the mixing depth.

Option B: The depth of each layer is determined dynamically using a "log-like" function. The function is defined such that the top of Layer 1 is at 20 m. The other layers with this option vary in both space and time.

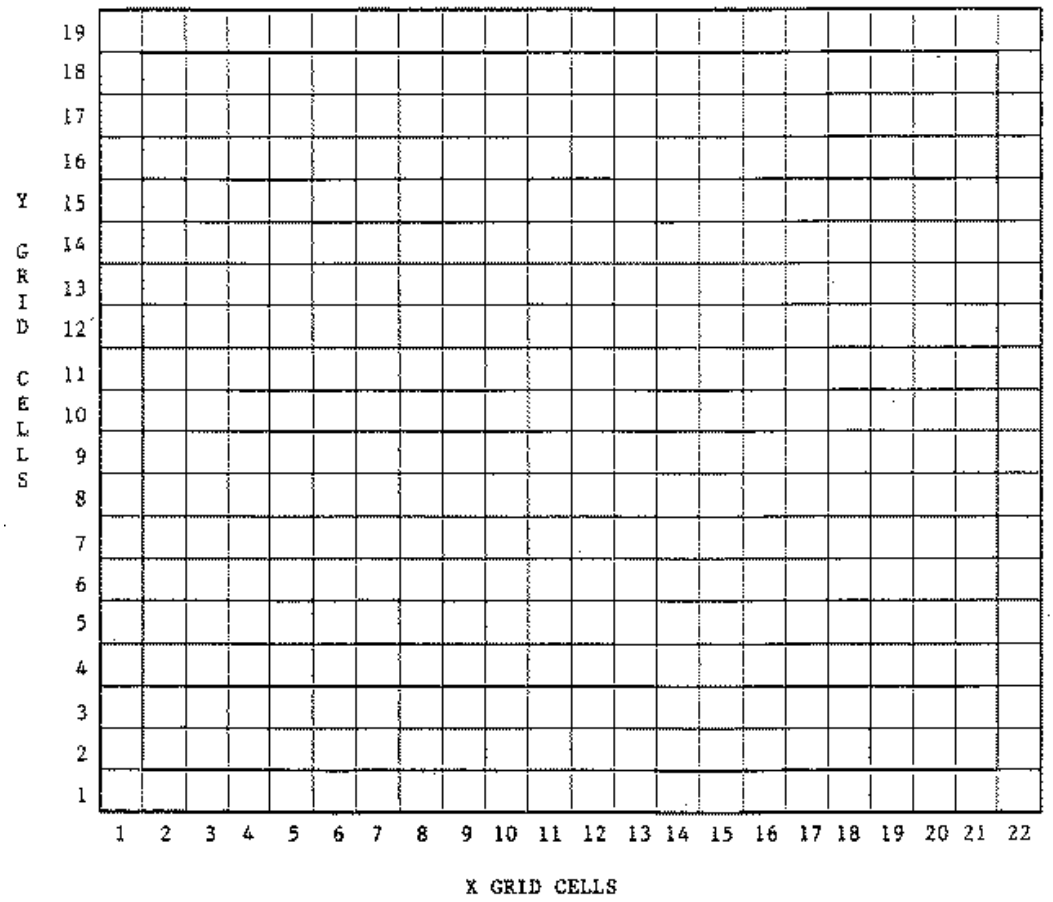

Figure 2.1-1: Schematic illustration of the CALGRID horizontal grid system for a 22×19 grid. The outer row and column of cells are inactive storage locations for the lateral boundary conditions. Only the interior portion of the grid is active (i.e., subject to advection, diffusion, chemistry, emissions injection, and dry deposition).

Option C: An arbitrary, fixed vertical system of user-specified layers is used. Layer 1 must be specified to be 20 m in depth. This option results in layers which are fixed in both space and time.

In the first option, the user specifies in the control file the total number of layers (NZ). the number of layers below the mixing height (NZL), the top of the modeling domain (ZTOP), and two sets of minimum/maximum values for layer depths (ZMINB, ZMAXB, ZMINA, ZMAXA) below and above the mixing height. The top of the first layer is fixed at 20 m to provide a grid point (i.e., at 10 m) that is within the atmospheric surface layer. Thus, with Option A, the layer depths, Δz, are:

$$\textbf{Layer 1:} \qquad \Delta z = 20m \tag{2.1-1}$$

$$\textbf{Layers 2,3,..NZL:} \quad \Delta z = \frac{z_i - 20}{\mathtt{NZL} - 1} \tag{2.1-2}$$

where z_i is the mixing height.

$$\textbf{Layers Above } z_i\textbf{:} \quad \Delta z = \frac{\mathtt{ZTOP} - z_i}{\mathtt{NZ} - \mathtt{NZL}} \tag{2.1-3}$$

The layer depths computed in this manner are then subject to the minimum/maximum values for layers below the mixing height (ZMINB, ZMAXB) and above the mixing height (ZMINA, ZMAXA). The purpose of the minimum/maximum conditions is to avoid numerical problems associated with very thin layers which can result from this scheme under low mixing heights conditions (e.g., $<$ 100 m). Except for the presence of the fixed, 20 m deep lowest layer, the level scheme generated by Option A is very similar to that employed by Reynolds et al. (1979) in the Airshed Model (UAM).

Option B involves a transformation of vertical coordinates to give a "log-like" spacing of the layers. The user must specify the total number of layers (NZ), the number of layers below the mixing height (NZL), the top of the modeling domain (ZTOP), and a minimum layer thickness (DZMIN).

The domain of the grid from the bottom face of the lowest cell, ZBOT, to the top of the modeling domain, ZTOP, is mapped into the coordinate, s, ranging from zero to one, by the relation

$$s = \frac{z - ZBOT}{ZTOP - ZBOT} \tag{2.1-4}$$

where ZTOP is specified by the user in the control file, and ZBOT is internally assigned a value of zero (i.e., ground level).

The variable s is then transformed to the variable, r:

$$r = \ln[1 + (e - 1)s] \tag{2.1-5}$$

where e is the base of natural logarithm (2.71828183), and $\ln$ signifies a natural logarithm.

A final transformation is made to ρ coordinates as

$$\rho = r[(l + p_1 + p_2)/(1 + p_1 r + p_2 r^2)] \tag{2.1-6}$$

where p_1 and p_2 are empirically determined coefficients computed internally to ensure the top of cell 1 is at $z = 20.0$m, and the top of cell NZL is at $z = z_1$.

This procedure involves two steps. In Step 1, simultaneous equations for p_1 and p_2 are determined and solved by substitution of $z = 20$m ($\rho = 1/\mathtt{NZ}$) and $z = z_i$ ($\rho = (\mathtt{NZL} + 1)/\mathtt{NZ}$) into equations (2.1-4) to (2.1-6).

In Step 2, r is determined for each cell face ($\rho = n/\mathtt{NZ}, n = 2, 3, \cdots, \mathtt{NZ} - 1$) from Eqn. (2.1-6), which is then solved for s (Eqn. (2.1-5)) and finally for z (Eqn. (2.1-4)).

The third option (C) for the vertical grid system is to use a fixed, arbitrary set of vertical layers. In this option, the user specifies the number of vertical layers (NZ), and the height of each cell face (NZ + 1 values). Note that the top face of the lowest cell must be 20 m. The other faces can be placed at arbitrary levels.

The three options for the vertical layer structure are illustrated in Figure 2.1-2. In the example, the model domain extends up to 5000 m, and a mixing height of 1000 m is assumed. Five layers are placed below the mixing height. The user inputs which would generate the layer structure are also shown in the figure. See Input Group 1 of the control file for more information.

Choice of a particular level spacing option should be guided by computational cost versus spatial resolution considerations. Option B represents a compromise between computational economy and reasonable near ground level resolution but users should be aware that the use of spatially varying. and/or time varying levels can be accompanied by increased interfacial fluxes of material and therefore increased numerical diffusion of concentrations in the vertical.

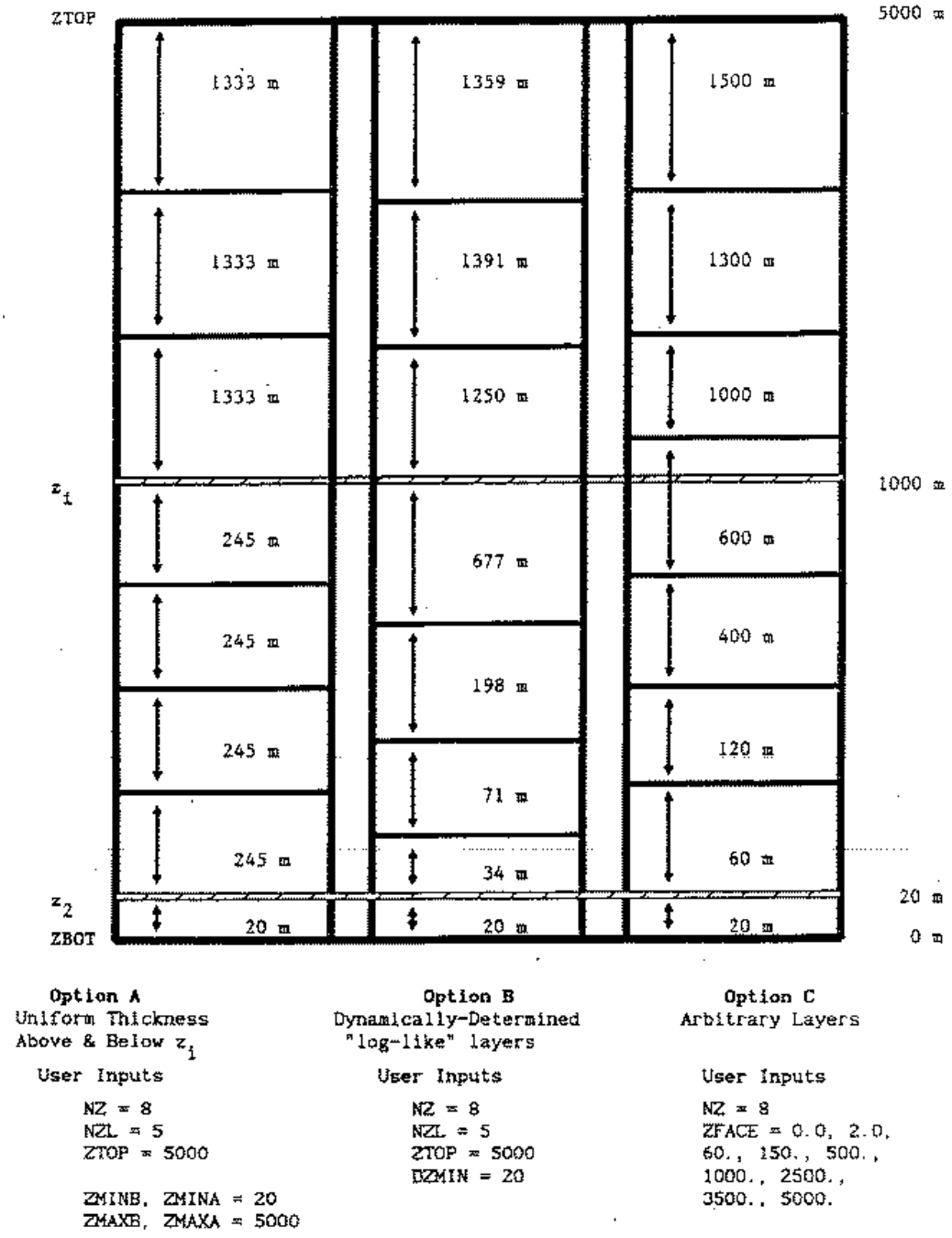

Figure 2.1-2: Schematic illustration of the CALGRID vertical grid system options.

2.2 Horizontal Advection and Diffusion

Horizontal Advection

The selection of a numerical scheme for the solution of the horizontal advection/diffusion equations for CALGRID is described in Yamartino et al. (1989). The method implemented in CALGRID is a high order chapeau function scheme. A nonlinear local filter, adapted from Forester (1977), is selectively applied to grid points, as needed, to eliminate the short wavelength numerical noise following in the wake of an advected distribution. This filtering and a subsequent mass borrowing scheme ensures that small negative concentrations are not generated.

The horizontal advection calculations are conducted in x-y planes of concentrations using a time step equal to one-half the basic model time step (see the variable NSUBTS in Input Group 1 of the control file). Within the advection module, advection of a 2-D plane of concentrations is accomplished as two sets of 1-D advection steps (1-D operator splitting involving x and y advection for a half time step before the full-time-step chemistry operator and followed by operator split and reversed y and x advection for the second half time Step).

The outer rows and columns of cells in the model grid are treated as boundary cells for which advection, chemistry, and other modeled processes are not computed. The active region of the grid consists of (NX-2)(NY-2) cells starting at grid cell (2,2) through (NX-1, NY-1).

The meteorological data required for the horizontal advection operation consists of 2-D gridded fields of u and v wind components for each CALGRID layer. The CALMET meteorological model generates u and v wind fields on a set of fixed meteorological grid levels.

These velocity components are then converted within CALGRID to the CALGRID coordinate system, which is assumed to correspond exactly with the meteorological model coordinate system in x and y and encompassed by it in z. In addition, the CALGRID vertical level structure can vary in time and space. The u and v Components within a vertical column are computed by a donor cell (or flux) weighting procedure to ensure air mass conservation.

This calculation depends on the definition of a simple matrix $f_{j,j'}$ describing the fractional portion of meteorological model level j which overlaps, or end up in, the CALGRID level j'. Defined in simple geometrical terms (i.e., lengths) for a system of NZ levels, this transfer matrix is computed by SUBROUTINE ZMATRIX

and is normalized such that

$$\sum_{j=1}^{\mathtt{NZ}} f_{j,j'} = 1 \quad \text{for all} \quad j'. \tag{2.2-1}$$

Thus, the mass conserving process of interpolation from a set of levels j onto a new set of vertical levels j' leads to the wind component $U_{j'}$, computed within SUBROUTINE WINDGRD as

$$u_{j'} = \sum_{j} f_{j,j'} \dot{u}_j. \tag{2.2-2}$$

with an identical equation for the v component.

Horizontal Diffusion

Several options are provided in CALGRID for the computation of lateral diffusivities. The user selects the lateral diffusivity formulation by setting a "method flag" in the CALGRID control file (see the variable KHMODE in Input Group 8). The four methods available in CALGRID are described below.

METHOD A:	Diffusivities within the boundary layer are determined based on the PGT stability class for each grid cell. Diffusivities above the boundary layer are determined by the control file variable DKHUP.
METHOD B:	Same as above except diffusivities are scaled by the wind speed.
METHOD C:	The Smagorinsky method is used to determine horizontal diffusivities.
METHOD D:	Results of Methods B and C are added.

In Method A, gridded fields of PGT stability class obtained from the meteorological data base are used to determine the lateral diffusivity for each grid cell within the boundary layer. The user inputs a set of six lateral diffusivities corresponding to PGT stability classes A through F. All grid cells above the boundary layer are assigned a constant, user-specified lateral diffusivity (see the variable DKHUP in Input Group 8 of the control file). These input variables can be set equal to zero for sensitivity testing of the model with no lateral diffusivity.

In the second method (B), the PGT stability-dependent boundary layer lateral diffusivities are multiplied by the horizontal wind speed in each grid cell. The lateral diffusivities above the boundary layer are determined by the product of the user-specified diffusivity, DKHUP, and the wind speed.

The Smagorinsky (1963) formulation, Method C, accounts for diffusion due to distortion or stress in the horizontal wind field.

$$
\begin{aligned}
K_h &= \alpha_0^2 |D| \Delta t \\
|D| &= \left[\left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)^2 + \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right)^2 \right]^{1/2}
\end{aligned}
$$

where K_h is the lateral diffusivity (m^2/s),
α_0 is a constant (≈ 0.28), and
Δt is the time step (sec).

This method yields diffusivities of zero for a uniform wind field and thus does not account for grid-scale turbulent processes. For plumes which are several kilometers or more across (i.e., Δx or greater), the Briggs (1973) parameterizations of lateral diffusion permit one to extract diffusivities which are constants times the transport wind speed ($(u^2 + v^2)^{1/2}$). These extracted constants are presented in Table 2.2-1 for both the "urban" and "rural" dispersion growth laws included in some short range regulatory models. Along with these values, a series of "rounded" values are included which increase by a factor-of-two per stability class as one proceeds from stable (F) through unstable (A). Given that the short-wavelength numerical diffusivity of the current chapeau function transport scheme is about $30u$ (m^2/sec), it can be concluded that E and F lateral diffusive transport cannot be realistically simulated, as these diffusivities are below the threshold of existing numerical diffusion. Subtracting a rounded numerical diffusivity values of $32u$ from the "rounded" values yields the final column of "suggested" values which a user may input via the CALGRID control file.

The user may also select whether the wind field stress induced diffusivity is to be added in to yield a total diffusivity (Method D). With this option, the lateral diffusivity computed using Method B (i.e., with wind speed scaling) is linearly added to the Smagorinsky diffusivity.

Table 2.2-1

Values Of The Horizontal "Grid Scale" Diffusivities***
Within The Boundary Layer As A Function of Stability Class

Diffusivity (m^2/sec)/u(m/sec)

Class	"Urban"*	"Rural"*	"Rounded"**	"Suggested"
A	128	242	256	224
B	128	128	128	96
C	60.5	60.5	64	32
D	32	32	32	0
E	15.1	18	16	0
F	15.1	8	8	0

* Extracted from Briggs (1973) dispersion curves as presented In U.S. EPA (1987).

** Based on a computed numerical diffusivity of about $30u$ (m^2/sec) (for $\Delta x = 2$ km, $\Delta t = 1800$s) for distributions covering more than 3 grid cells.

*** See the array `DKHSTB` in Input Group 8 of the control file.

2.3 Vertical Advection and Diffusion

Vertical Advection

The `CALGRID` modeling system operates In a terrain-following coordinate system:

$$Z = z - h_t \tag{2.3-1}$$

where Z is the terrain following vertical coordinate (m),
z is the Cartesian vertical coordinate (m), and
h_t is the terrain height (m).

The vertical velocity, W, in the terrain following coordinate system is

$$W = w - u\frac{\partial h_t}{\partial x} - v\frac{\partial h_t}{\partial y} \tag{2.3-2}$$

where w is the physical vertical wind component (m/s) in Cartesian coordinates, and u, v are the horizontal wind components (m/s).

The `CALGRID` model reads hourly three-dimensional fields of the u, v and W wind components in a separate, fixed meteorological grid system. The u, v,

components are defined at the center of each grid cell, whereas the W components are defined at the vertical cell faces.

As with the u and v components, the W components are transformed within CALGRID from the CALMET meteorological model's fixed vertical level scheme to the potentially space- and time-varying CALGRID vertical level scheme. Unlike the flux-weighting invoked for the u and v components, mass conserving computation of the W component at the CALGRID vertical cell faces involves simple linear interpolation between the two neighboring meteorological grid-cell-face values.

The terrain-following vertical velocities are used to determine the advective flux through each of the vertical cell faces. A redistribution of pollutant mass among the model layers is also required when the dynamically varying layer option is used in the model. This is due to both horizontal advective fluxes associated with spatial changes in the layer heights as well as the explicit time variation of the layer heights.

The methods used to accomplish this pollutant redistribution include:

1. A mass conserving interpolation of pollutant material to the new set of vertical levels after the vertical advection step is completed to account for the time variation in the level heights
2. Tracking of horizontal advective fluxes $\left(u\frac{\partial z}{\partial x}, v\frac{\partial z}{\partial y}\right)$, on a species by species basis and a subsequent reappointment of this mass to account for spatial changes In the layer heights.

The procedures and numerical methods involved in vertical advection and pollutant redistribution due to the changes in the layer heights are described in more detail in the companion model formulation report (Yamartino et al., 1989).

Vertical Diffusion

The vertical diffusivities, K_z, used in CALGRID are based on convective scaling in the daytime boundary layer and local or z-less scaling in the nighttime boundary layer. Gridded fields of mixing height, z_i, surface friction velocity, u_{*_0}, Monin-Obukhov length, L and convective velocity scale, w, are required by CALGRID in the computation of K_z.

In the convective boundary layer ($L < 0$) vertical diffusivities are computed at cell faces as follows:

Surface Layer ($z/z_i \leq 0.1;\ -z/L < 1.0$)

$$K_z = 0.4u_{0*}z/\phi_h(z/L) \tag{2.3-3}$$

where $\phi_h(z/L) = 0.74(1 - 9z/L)^{-1/2}$, and z is the height of the cell face (m) above the ground.

Free Convection Layer ($z/z_i \leq 0.1;\ -z/L > 1$)

$$K_z = w_* z \tag{2.3-4}$$

Near neutral upper layer ($0.1 < z/z_i \leq 1;\ -z_i/L < 10$)

$$K_z = 0.04 u_{0*} z_i / \phi_h(0.1 z_1/L) \tag{2.3-5}$$

Mixed layer ($0.1 < z/z_i \leq 1.0;\ -z_i/L > 10$)

$$K_z = 0.1 w_* z_i \tag{2.3-6}$$

Layer above the mixing height ($z/z_i > 1.0$)

$$K_z = (K_z)_{\min} \tag{2.3-7}$$

$(K_z)_{\min}$ is a user input (see Input Group 8 of the control file).

The vertical diffusivity at the top of the model domain, DKZTOP, is also a user input, with a default value of zero.

In the stable boundary layer ($L > 0$), the following equations are used to compute the vertical diffusivity.

Surface layer ($z/z_i \leq 0.1$; $(z_i - z)/\Lambda < 10$)

$$K_z = 0.4 u_* z / \phi_h(z/L) \tag{2.3-8}$$

where $\phi_h(z/L) = 0.74 + 4.7 z/L$

Near neutral upper layer ($0.1 < z/z_i < 1.0$; $z_i/L < 1$)

$$K_z = 0.04 u_{0*} z_i / \phi_h(0.1 z_i/L) \tag{2.3-9}$$

For local and z-less scaling, the local friction velocity, u_*, local sensible heat flux, $\overline{w\theta}$, and local Monin-Obukhov length, Λ, are computed from their surface values.

$$\overline{w\theta} = \overline{w\theta_0}(1 - z/z_i) \quad \text{(2.3-10)}$$

$$\Lambda = -\frac{u_*^3}{k(g/T)\overline{w\theta}} \quad \text{(2.3-11)}$$

Local scaling layer ($0.1 < z/z_i$; $z_i/L > 1$; $z/\Lambda < 1$)

$$K_z = 04u_* z/\phi_h(z/\Lambda) \quad \text{(2.3-12)}$$

z-less scaling layer ($0.1 < z/z_i$; $z_i/L > 1$; $1 < z/\Lambda < (z_i/\Lambda) - 10$)

$$K_z = 0.4u_*\Lambda \quad \text{(2.3-13)}$$

Intermittency layer and layer above the mixing height ($z/\Lambda > (z_i/\Lambda) - 10$)

$$K_z = (K_z)_{\min} \quad \text{(2.3-14)}$$

$(K_z)_{\min}$ is a user input (see Input Group 8 of the control file).

2.4 Dry Deposition

Three options are provided in the `CALGRID` model for treating dry deposition.

- Full treatment of spatially and temporally varying gas/particle deposition rates predicted by a resistance deposition model.
- User-specified 24-hour cycles of deposition velocities for each pollutant. This option will allow a "typical" time dependence of deposition to be incorporated, but will not include any spatial dependencies.
- No dry deposition.

The user specifies a flag in the control file for each pollutant, and this flag determines if dry deposition is treated and the specific method used to compute the deposition velocities (see Input Group 3, Section 4.1.1).

The resistance deposition model is described in Sections 2.4.1 and 2.4.2. If the resistance deposition model is used, the user must input values for several parameters describing the characteristics of the pollutant (e.g., solubility, reactivity, diffusivity for gases. the size distribution for particles) (see Input Groups 5 and 6) which are used in the computation of the resistances. In addition, several reference parameters and a flag indicating the state of unirrigated vegetation (i.e., stressed, unstressed, or inactive) are required (see Input Group 7).

If any pollutant is flagged as using "user-specified" deposition velocities, the user must prepare a data file with a 24-hour diurnal cycle of deposition velocities for each flagged species (see Section 4.1.10).

2.4.1 Resistance Deposition Model For Gases

A commonly used measure of deposition is the deposition velocity, defined as:

$$v_d = F/C_S \tag{2.4-1}$$

where, v_d is the deposition velocity (m/s),
F is the pollutant deposition flux (g/m^2/s), and,
C_S is the pollutant concentration (g/m^3).

At the reference height, z_S, the deposition velocity for gases is expressed (Wesely and Hicks, 1977; Hicks, 1982) as the inverse of a sum of resistances.

$$v_d = (r_a + r_b + r_c)^{-1} \tag{2.4-2}$$

where r_a is the atmospheric resistance (s/m) through the surface layer,
r_d is the deposition layer resistance (s/m), and,
r_c is the canopy (vegetation layer) resistance (s/m).

Atmospheric Resistance

The atmospheric resistance is obtained by integration of the micrometeorological flux-gradient relationships (Wesely and Hicks, 1977):

$$r_a = \frac{1}{ku_*}[\ln(z_S/z_0) - \phi_H] \tag{2.4-3}$$

where z_S is the reference height (m),
z_0 is the surface roughness length (m),
k is the von Karman constant (≈0.4),
u_* is the friction velocity (m/s),
ϕ_H is a stability correction term, and,
L is the Monin-Obukhov length (m).

The stability correction term accounts for the effects of buoyancy on the eddy diffusivity of the pollutant. It is assumed that the pollutant transfer is similar to that for heat (Wesely and Hicks, 1977). A gridded field of surface roughness lengths is passed to the model in the output file of the meteorological model, CALMET. In CALMET, the surface roughness length is either estimated from the predominant land use of each grid cell, or, if available, based on actual values entered by the user. Over water, due to the effect of the wind on wave height, the surface roughness length varies as a function of wind speed, and is computed internally within CALGRID. Hosker (1974) parameterizes z_0 over water as

$$z_0 = 2.0 \times 10^{-6} u^{2.5} \tag{2.4-4}$$

where u is the wind speed (m/s) at 10 m.

Because the concentration in the lowest layer is a vertical average through the cell depth, Eq. (2.4-3) must be vertically integrated in order to provide the proper cell resistance. Pleim et al. (1984) found that a good approximation of the integrated expression can be obtained by substituting z in Eq. (2.4-3) with

$$z = \frac{\Delta z - z_1}{e} + z_1 \tag{2.4-5}$$

$$\Delta z = z_2 - z_1 \tag{2.4-6}$$

where Δz is the depth (m) of the lowest grid cell,
z_1, z_2 are the bottom and top face heights (m) of the first grid cell, and,
e is the base of natural logarithms (2.7182818).

Deposition Layer Resistance

Due to the importance of molecular diffusion to the transport through the laminar deposition layer, the deposition layer resistance for gaseous pollutants is parameterized in terms of the Schmidt number:

$$r_d = d_1 S_c^{d_2} / (k u_*) \tag{2.4-7}$$

where S_C is the Schmidt number (v/D),
v is the kinematic viscosity of air (m^2/s),
D is the molecular diffusivity of the pollutant (m^2/s), and,
d_1, d_2 are empirical parameters.

Experimental studies summarized by Hicks (1982) suggest a range of values for the empirical variables of 1.6 to 16.7 for d_1 and 0.4 to 0.8 for 1 d_2. Intermediate values of $d_1 = 5$, and $d_2 = 2/3$ are recommended based on Shepherd (1974), Slinn et al. (1978), and Hicks (1982).

Canopy Resistance

The canopy resistance is the resistance for gases in the vegetation layer. There are three main pathways for uptake/reaction of the pollutant within the vegetation or surface:

1. Transfer through the stomatal pore and dissolution or reaction in the mesophyll cells.
2. Reaction with or transfer through the leaf cuticle.
3. Transfer into the ground/water surface.

In the resistance model, these pathways are treated as three resistances in parallel.

$$r_c = [\texttt{LAI}/r_f + \texttt{LAI}/r_{\text{cut}} + 1/r_g]^{-1} \quad \text{(2.4-8)}$$

where r_f is the internal foliage resistance (s/m) (Pathway 1),
r_{cut} is the cuticle resistance (s/m), (Pathway 2),
r_g is the ground or water surface resistance (s/m), (Pathway 3), and,
LAI is the leaf area index (ratio of leaf surface area divided by ground surface area). The LAI is specified in the model as a function of land use type.

The first pathway is usually the most important for uptake of soluble pollutants in vegetated areas. The internal foliage resistance consists of two components:

$$r_f = r_s + r_m \quad \text{(2.4-9)}$$

where r is the resistance (s/m) to transport through the stomatal pore, and
r_m is the resistance (s/M) to dissolution or reaction of the pollutant in the mesophyll (spongy parenchyma) cells.

Stomatal action imposes a strong diurnal cycle on the stomatal resistance, and, due to its important role for gaseous, soluble pollutants such as SO_2, on the deposition velocity. Stomatal opening/closing is a response to the plant's competing needs for uptake of CO_2 and prevention of water loss from the leaves. The stomatal resistance can be written (O'Dell et al., 1977) as:

$$r_s = p/(bD) \tag{2.4-10}$$

where p is a stomatal constant ($\approx 2.3 \times 10^{-8}$m^2),
b is the width of the stomatal opening (m), and,
D is the molecular diffusivity of the pollutant (m^2/s).

The width of the stomatal opening is a function of the radiation intensity, moisture availability, and temperature. The variation of b during periods when vegetation is active can be represented (Pleim et al., 1984) as:

$$b = b_{\max}[S/S_{\max}] + b_{\min} \tag{2.4-11}$$

where $b_{\max}$ is the maximum width (m) of the stomatal opening ($\approx 10 \times 10^{-6}$m).
$b_{\min}$ is the minimum width (m) of the stomatal opening ($\approx 0.1 \times 10^{-6}m$),
S is the solar radiation (W/m^2) received at the ground, and
$S_{\max}$ is the solar radiation (W/m^2) at which full opening of the stomata occur.

However, during periods of moisture stress, the need to prevent moisture loss becomes critical, and the stomata close. It can be assumed that $b = b_{\min}$ for unirrigated vegetation under moisture stress conditions. when vegetation is inactive (e.g., during the seasonal dry periods in much of California), the internal foliage resistance becomes very large, essentially cutting off Pathway 1. In `CALGRID`, the state of the unirrigated vegetation is specified as one of these states (A) active and unstressed, (B) active and stressed, or (C) inactive.

The effect of temperature on stomatal activity has been reviewed by Pleim et al. (1984). The most significant effects are due to temperature extremes. During cold periods ($T < 10^o$ C), metabolic activity slows, and b is set equal to $b_{\min}$. During hot weather conditions ($T > 35^o$ C), the stomata mm are fully open ($b = b_{\max}$) to allow evaporative cooling of the plant (assuming the vegetation is in state A - active and unstressed). These temperature effects provide additional bounds on the value of r_f given by Eq. (2.4-9).

Mesophyll Resistance

The mesophyll resistance depends on the solubility and reactivity of the pollutant. It is an input parameter supplied to the deposition model for each gaseous species. O'Dell et al. (1977) estimate the mesophyll resistance for several pollutants. For soluble pollutants such as HF, $S0_2$, Cl_2 and NH_3, $r_m \approx 0.0$. The mesophyll resistance can be large for less soluble pollutants such as NO_2 ($\approx$ 500 s/cm) and NO (9400 s/cm). For other pollutants, r_m can be estimated based on the solubility and reactivity characteristics of the pollutant.

Cuticle Resistance

The second pathway for deposition of gases in the vegetation layer is via the leaf cuticle. This includes potential direct passage through the cuticle or reaction of the pollutant on the cuticle surface. Hicks (1982) notes that measurements of SO_2 deposition to wheat (Fowler and Unsworth, 1979) show significant cuticle deposition. However, Hosker and Lindberg (1982) suggest that passage of gases through the cuticle is negligible. Therefore, the cuticle deposition is likely to be controlled by the pollutant reactivity. Pleim et al. (1984) parameterize r_{cut} as a function of the pollutant reactivity of the depositing gas relative to the reference values for $S0_2$.

$$r_{\text{cut}} = (A_{\text{ref}}/A) r_{\text{cut}}(\text{ref}) \tag{2.4-12}$$

where A is the reactivity parameter for the depositing gas,
A_{ref} is the reference reactivity of SO_2 ($\approx$ 8.0), and,
$r_{\text{cut}}(\text{ref})$ is the empirically determined reference cuticle resistance (s/m) of SO_2

Pleim et al. (1984) suggest $r_{\text{cut}}(\text{ref})$ is about 17 s/cm. Reactivity values for other pollutants are estimated at 8.0 (NO_2), 15.0 (O_3), 18.0 (HNO_3), and 4.0 (PAN).

Ground/Water Resistance

The third pathway through the "vegetation layer" involves deposition directly to the ground or water surface. In moderately or heavily vegetated areas, the internal foliage and cuticle resistances usually control the total canopy resistance. However, in sparsely vegetated area of California, deposition directly to the surface may be an important pathway. Over water, deposition of soluble pollutants can be quite rapid.

The ground resistance, r_g over land surfaces can be expressed (Pleim et al., 1984) relative to a reference value for SO_2:

$$r_g = (A_{\text{ref}}/A) r_g(\text{ref}) \tag{2.4-13}$$

where $r_g(\text{ref})$ is the reference ground resistance of SO_2 ($\approx$ 5 s/cm).

Slinn et al. (1978) parameterize the liquid phase resistance of the depositing pollutant as a function of its solubility and reactivity characteristics. Their results can be expressed as:

$$r_g = H/(\alpha_* d_3 u_*) \tag{2.4-14}$$

where H is the Henry's law constant, which is the ratio of gas to liquid phase concentration of the pollutant, ($H \approx 4 \times 10^{-2}$ (SO_2), 4×10^{-7} (H_20_2), 8×10^{-8} (HNO_3), 2×10^{0} (0_3), 3.5×10^{0} (NO_2), 1×10^{-2} (PAN), and 4×10^{-6} (HCHO)),

α_* is a solubility enhancement factor due to the aqueous phase reactivity of the pollutant ($\alpha_* \approx 10^3$ for SO_2, ≈ 1 for CO_2), and,

d_3 is a constant ($\approx 4.8 \times 10^{-4}$).

The values for α_*, H, and other dry deposition parameters for gases are specified in Input Group 4 of the control file. Values for these parameters, which were used in the initial testing of CALGRID, are shown on Page 4-10. However, these are preliminary values which may need to be updated as new data become available.

2.4.2 Deposition of Particulate Matter

In the CALGRID model, H_2SO_4 is treated as particulate sulfate for purposes of computing its rate of dry removal. Because particulate matter does not interact with vegetation in the same way as gaseous pollutants, particle deposition velocities are commonly expressed only in terms of r_a, r_d and a gravitational settling term. The resistance in the vegetation layer (r_c) is not a factor because once penetrating the deposition layer, particles are usually assumed to stick to the surface (e.g., Voldner et al., 1986). Therefore, their behavior is similar to highly soluble/reactive gases with $r_c \approx 0$. Based on an assumption of steady-state conditions, the deposition velocity for particles can be expressed (Slinn and Slinn, 1980; Pleim et al., 1984) as:

$$v = (r_a + r_d + r_a r_d v_g)^{-1} + v_g \tag{2.4-15}$$

where v_g is the gravitational settling speed (m/s) of the particle.

The atmospheric resistance, r_a is obtained from Eq. (2.4-3). There are three major mechanisms for transport of particles across the deposition layer. Small particles ($< 0.1\mu$m diameter) are transported through the laminar deposition layer primarily by Brownian diffusion. This process becomes less efficient as the particle diameter increases. Particles in the 2-20 μm diameter range tend to penetrate the deposition layer by inertial impaction. The stopping time, t, defined as the settling velocity divided by the acceleration due to gravity, is a measure of tendency of a particle to impact. Inertial impaction is most effective in the 2-20 μm diameter range. Larger particles are dominated by gravitational settling effects. The effect of the terms involving v_g in Eq. (2.4-15) always is to increase the deposition velocity. Particles in the range of 0.1-2 μm diameter range. such as sulfate, have very small settling velocities and are not efficiently transported across the deposition layer by either the Brownian diffusion or the inertial impaction mechanism. As a result, these particles have the lowest deposition velocities.

The deposition layer resistance can be parameterized (e.g., Pleim et al. 1984) in terms of the Schmidt number ($Sc - \upsilon/D$, where υ is the viscosity of air, and, for particles, D is the Brownian diffusivity of the pollutant in air) and the Stokes number ($St = (v_g/g)(u_*^2/\upsilon)$, where v_g is the gravitational settling velocity and g is the acceleration due to gravity).

$$r_d = (Sc^{-2/3} + 10^{-3/St})^{-1} u_*^{-1} \tag{2.4-16}$$

The diffusivity of a particle in air, D, is a function of the particle size. Smaller particles tend to be more efficiently transported by Brownian motion, and therefore have higher diffusivities. The Stokes number is a measure of the likelihood of impaction of the particle. It increases with increasing particle size.

The gravitational settling velocity is a function of the particle size, shape, and. density. For spheres, the settling velocity is given by the Stokes equation:

$$v_g = [(d_p)^2 g(\rho_p - \rho_g)C]/(18\upsilon) \tag{2.4-17}$$

where d is the particle diameter (m)
ρ_p is the particle density (g/m^3),
ρ_g is the air density (g/m^3), and,
C is the Cunningham correction for small particles. This correction given by:

$$C = 1 + (2\lambda/d_p)[a_1 + a_2 e^{-a_3 d_p/\lambda}] \tag{2.4-18}$$

where A is the mean free path of air molecules (6.53×10^{-6} cm), and
a_1, a_2, a_3 are constants (1.257, 0.40, 0.55, respectively).

Because of the sensitivity of the deposition velocity to particle size, the effective deposition velocity is computed for a number of individual size categories, and then weighted by the actual size distribution. The particle size distribution is specified in terms of the geometric mass mean diameter and geometric standard deviation of the distribution. For sulfate, the geometric mass mean diameter is approximately 0.5 μm with a geometric standard deviation of approximately 2 μm.

2.5 Plume Rise

The plume rise of stationary and mobile buoyant point sources is computed internally within the `CALGRID` model. The effects of plume buoyancy, stable atmospheric stratification, and partial penetration into an elevated inversion layer are included using the plume rise relationships of Briggs (1975).

For neutral and unstable conditions at the surface, the final plume rise is computed as the minimum of two values:

$$\Delta h = \text{minimum}(\Delta h_1, \Delta h_2) \tag{2.5-1}$$

The neutral, bent-over plume rise equation of Briggs (1975) is used for Δh_1.

$$\Delta h_1 = \frac{1.6 F^{1/3} X_f^{2/3}}{u} \tag{2.5-2}$$

where F is the buoyancy flux (m^4/s^3),
X_f is the distance to final plume rise (m),
u is the wind speed (m/s) in the layer containing the stack top, and,
Δh_1 is the plume rise (m).

The distance to final plume rise is:

$$X_f = 3.5 X^* \tag{2.5-3}$$

where

$$X^* = \begin{cases} 14 F^{5/8}, F \leq 51.6 m^4/s^3 & (2.5\text{-}4) \\ 34 F^{2/5}, F > 51.6 m^4/s^3 & (2.5\text{-}5) \end{cases}$$

The threshold for the use of Eqns. (2.5-4) and (2.5-5) is set so that the values of X^* match at the crossover point.

The effect of the elevated stable layer above the convective boundary layer is evaluated using the Briggs partial penetration equation.

$$\Delta h_2 = \left(1.8 Z_b^3 + \frac{3F}{\beta'^2 u S}\right)^{1/3} \tag{2.5-6}$$

where Z_b is the distance from the top of the stack, h_S, to the mixing height (Z_i) (i.e., $Z_b = Z_i - h_S$),
β' is an entrainment parameter,
S is a stability parameter ($S = (g/T_a)(d\theta/dz)$),
g is the acceleration due to gravity (m/s^2),
T_a is the ambient air temperature (^{o}K), and
$d\theta/dz$ is the potential temperature lapse rate in the stable layer above the mixing height (^{o}K/m).

The entrainment parameter, β', is assigned a value of 0.41314 in order that the plume rise match the stable rise equation, Eqn. (2.5-8), for stacks imbedded within the stable layer (i.e., $h_S > Z_i$). A minimum stack height wind speed of 1 m/s is used in Eqns. (2.5-2) and (2.5-6) to avoid numerical problems.

During stable conditions at the surface, the final plume height is computed as a minimum of Briggs stable bent-over and vertical plume rise values.

$$\Delta h = \text{minimum}(\Delta h_{s1}, \Delta h_{s2}) \tag{2.5-7}$$

$$\Delta h_{s1} = 2.6 \left(\frac{F}{uS}\right)^{1/3} \tag{2.5-8}$$

$$\Delta h_{s2} = \frac{5F^{1/4}}{S^{3/8}} \tag{2.5-9}$$

2.6 Emission Injection

Point Source Emissions

The pollutant emissions from buoyant point sources is injected into one or more CALGRID model layers based on the height of the stack, final plume rise, and the overlap of the plume with the model layers.

The procedure involves the computation of (1) buoyant plume rise (Δh), (2) vertical plume depth (D) assuming a top-hat vertical distribution ($D = 2(0.6\Delta h)$),

and (3) fraction of the pollutant mass within each CALGRID vertical layer proportional to the fraction of the plume contained within each layer. This procedure is illustrated schematically in Figure 2.6-1.

In the example, the point source emissions are distributed into the CALGRID two layers (a fraction $d_3/(d_2 + d_3)$ into layer 3, and $d_2/(d_2 + d_3)$ into layer 2). Note that $d_2 + d_3$ is equal to the top hat plume depth ($1.2\Delta h$).

The plume rise and vertical distribution of emissions are computed on an hourly basis for each point source for the particular grid column containing the stack.

Area Source Emissions

Area source emissions are injected into CALGRID layers using a distribution function defined in the control file (see Input Group 1, Section 4.1.1). The user specifies the fraction of the area source emissions to be distributed among each of a number of "emission layers" The partitioning of the area source emissions into the various CALGRID model layers is computed hourly based on the overlap of each emissions layer with the CALGRID layers.

The procedure is illustrated in Figure 2-6.2. The default emissions distribution function calls for 75% of the area source emissions to be injected below 50 m and 25% between 50-100 m. In the example, the first three CALGRID model layers extend from 0-20 m, 26-80 m, and 80-160 m. Distributing the area source emission proportionally to the overlay of each emission layer with the CALGRID layers results in 30%, 60%, and 10% of the mass being injected into CALGRID layers 1, 2, and 3, respectively.

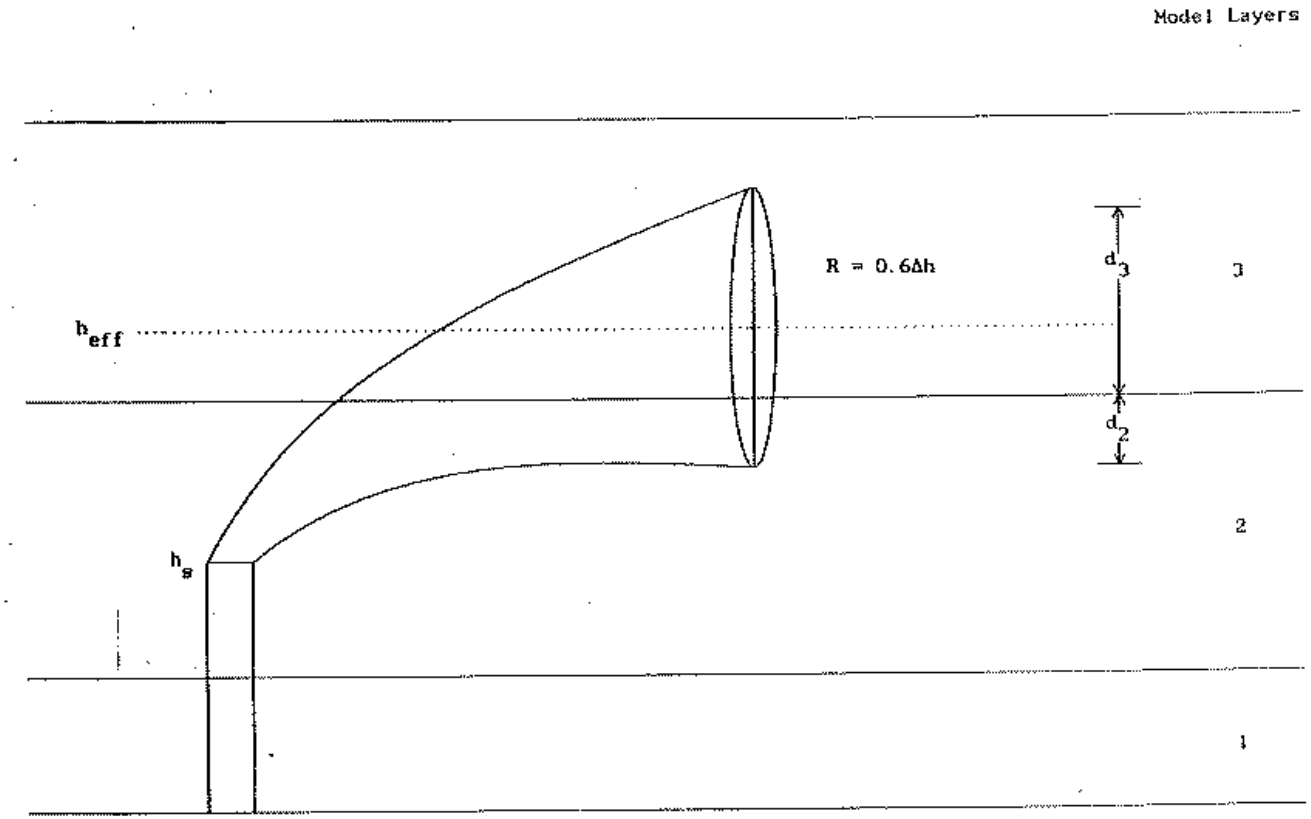

Figure 2.6-1: Schematic showing distribution of point source emissions between two layers. Fractions of pollutant mass injected into layers 2 and 3 are $d_2/(d_2+d_3)$ and $d_3/(d_2+d_3)$, respectively. The top hat plume diameter is $D = 2(0.6\delta h) = d_2 + d_3$. The stack height is h_s, the effective plume height is h_{eff}, the plume radius is R, and the plume rise is δh.

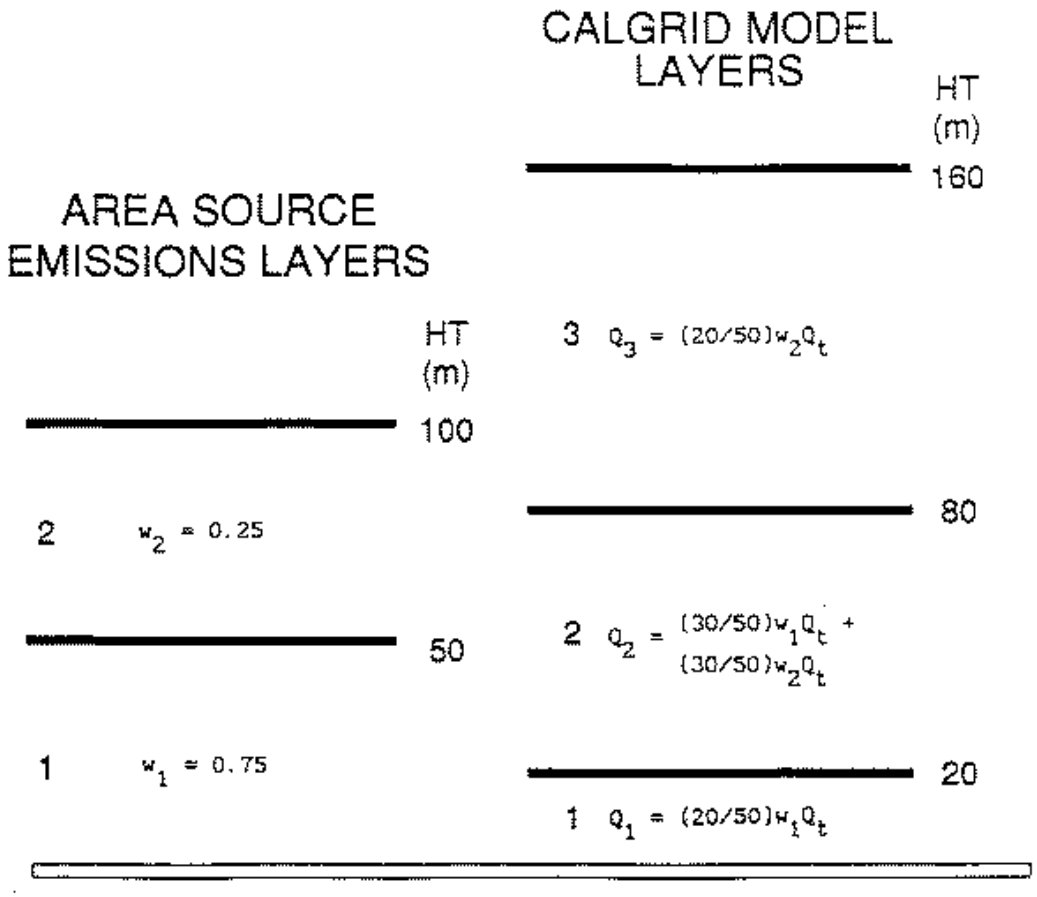

Figure 2.6-2: Schematic showing the distribution of area source emissions among CALGRID model layers. The area source distribution function calls for 75% of the total area source mass, Q_t, to be distributed below 50 m, and 25% between 50–100 m. Because of the CALGRID model layer structure in this example, this results in 30%, 60%, and 10% of the area source mass being injected in CALGRID layers 1 (0–20 m), 2 (20–80 m), and 3 (80–100 m), respectively.

2.7 Chemistry

Current Chemical Mechanism in CALGRID

The chemical integration procedures and the CALGRID model have been tested to date using the Carter chemical mechanism identified as LMPBE22l. This mechanism is described in detail by Carter (1988) and is quite similar to the Lurmann, Lloyd, and Atkinson (LLA) mechanism (1986). This mechanism contains 50 chemical species and 102 chemical reactions. Most of the active and buildup species involved in this scheme are listed in Table 2.7-1. It uses 2 alkanes, 2 aromatics, and 2 alkenes in the lumping of the hydrocarbons; two concentrations (O_2, m) are treated as constants, and ten species, OH, O, O('D), RO_2-R^o, RO_2-N^o, $R_2O_2^o$, RO_2-XN, $HOCOO^o$, NO_2^o, and O_3OL-SB^o, are treated under the pseudo steady-state approximation. Also, a unit photon concentration, hν, is held fixed as a parameter, whereas the H_2O concentration is updated on an hourly and cell-by-cell basis. The actual mechanism is listed (as lines 197-333 of the input file LMPBE221.MOD) in Table 4.1.11-2.

Within the treatment of the chemical mechanism, the thermal reactions are specified using an extended Arrhenius kinetics expression, i.e.,

$$k = A * (\texttt{TEMP}/\texttt{TREF}) * *B * \exp[-E_a/0.0019877 * \texttt{TEMP}) \qquad (2.7\text{-}1)$$

where TEMP is the ambient temperature in K, A is the Arrhenius pre-exponential factor, E_a is the activative energy in kcal/mol, and B is a unitless quantity. Thermal reactions which are not at their high pressure limit, are treated using the Troc falloff expression (see Carter (1988))

The rate constants for the photolysis reactions are calculated using the intensity and spectral distribution of the light source, and the absorption coefficients and quantum yields of the photolysis reactions, i.e.,

$$k_{A\nu} = \int_{\infty}^{0} \sigma[\lambda, T(h)]\, I[\lambda, N(T), \mathbf{X}]\, d\lambda \qquad (2.7\text{-}2)$$

where σ is the wavelength (σ) and temperature ($T(h)$) dependent absorption cross section coefficient, ϕ is the wavelength and temperature dependent quantum yield, and I is the actinic irradiance corresponding to the atmospheric state N at spatial location $\mathbf{X}$.

TABLE 2.7-1

Listing of Active and Buildup Species in the `LMPE22l.MOD` Chemical Mechanism

Model Species	**Description**
	Inorganic Species
O3	Ozone
NO	Nitric Oxide
NO2	Nitrogen Dioxide
NO3	Nitrogen Trioxide
N2O5	Nitrogen Pentoxide
HONO	Nitrous Acid
HONO2	Nitric Acid
HO2NO2	Peroxy Nitric Acid
HO2	Hydroperoxy Rad.
H2O2	Hydrogenperoxide
SO2	Sulfur Dioxide
H2SO4	Sulfuric Acid
	Generalized peroxy or hydroperoxy species
RO2	Total Alkly Peroxy
RCO3	Total Acyl Peroxy
-OOH	Lumped Rydropero
RO2-HO2 Prod.	Products
RO2-RO2 Prod.	Products
	Organic intermediate or reactive products
CO	Carbon Monoxide
HCHO	Formaldehyde
CCHO	Acetaldehyde or Lumped Aide
PAN	Peroxyacetly Nitrate
MEK	Lumped Ketones
MGLY	Methly Glyoxal
CRES	Cresol
AFG2	Aromatic Frags
RNO3	Lumped Org-Nitra.
	Alkanes, aromatics, alcohols, ethers, etc.

TABLE 2.7-1

Listing of Active and Buildup Species in the LMPE22l.MOD Chemical Mechanism

Model Species	Description
AAR1	Lumped Alkane and Aromatics
AAR2	Lumped Aikane and Aromatics
AAR3	Lumped Alkane and Aromatics
AAR4	Lumped Alkane and Aromatics
	Alkenes
ETHE	Ethene
OLE1	Lumped Alkenes

The absorption coefficients and quantum yields are input as part of the chemical mechanism (i.e., LMPBE221.MOD) The photolysis constants at ground level are calculated in the subroutine NEWPHK by numerically integrating Eq. (2.7-2). The photolysis rate constants as a function of height are calculated by empirical correlations using the surface values and the change in solar actinic flux with height, as shown in Carmichael et al. (1986). The solar intensity Is based on the work of Peterson (1976) and calculated based on Julian date, time and latitude.

The water vapor concentration as a function of height is calculated according to the polynomial expression of Richards (1971). This calculation is performed in subroutine WATCON.

Selection of Chemical Solver Methodology

The CALGRID model offers the user a choice of two numerical methods for the time integration of the chemical mechanism: the hybrid method and the Quasi Steady State Analysis (QSSA) method. Both of these methods are many times faster than the implicit Gear method, which is the standard or reference method,

The hybrid solver was developed by McRae et al. (1982) and is based on a second-order, predictor-integrated corrector scheme (Young and Boris, 1977). The QSSA technique, developed by Hesstvedt, Hov and Isaksen (1978), actually breaks the species into three groups based on their time rate of change relative to the basic time step. Very rapidly varying species are solved via the algebraic equations resulting from the steady-state assumption, moderately varying species are integrated via an analytic solution which assumes slowly varying species concentrations are

constant, and the slowest varying species (and hence the entire system) are marched via an explicit Euler method.

With appropriate species lumping to ensure mass conservation of sulfur (S) and nitrogen (N), the QSSA method has proven to be faster and maintain better S and N conservation than the hybrid scheme for the chemical scheme, LMPBE22l, initially installed in CALGRID. However, the implementation of alternative chemical mechanisms into CALGRID requires expert judgments and numerical experiments to properly allocate species between the three QSSA rate categories to ensure optimal QSSA performance. Thus, the hybrid solver option has been retained to permit such comparative studies subsequent to a chemical mechanism change.

Preparation of Emissions-Specific Chemical Parameters

The CALGRID model also makes use of Carter's scheme for the preparation of the emissions data, so that the emissions are consistent with the chemical mechanism selected (i.e., classifying the hydrocarbon emissions according to the lumping scheme used), and adjusts emissions specific parameters (e.g., emissions weighted reaction rates) of the chemical mechanism. This information is contained in a model input file, currently called CALBE221.RXP.

The flow of data and program relationships involved in the generation of the emissions specific .RXP CALGRID input files is displayed in Figure 2.7-1. The CALBE221.RXP file is an output file for Carter's PREPEMIT program. This file is read only once at the beginning of the CALGRID simulation. This data set must be changed if either the emissions or the chemical reaction mechanism is changed. The procedures involved in the development of a .RXP file are described in detail by Carter (1988). The file structure is described in more detail in Section 4.1.12.

Inclusion of Alternative Chemical Mechanisms into the CALGRID Model

The CALGRID model has been structured so that the chemical mechanism can be modified or exchanged easily and without the need to perform extensive recoding. To facilitate the ease of modifying the chemical mechanism, the procedures developed by Carter (1988) are incorporated into the model. The primary feature of this treatment is that the chemical mechanism is read as an input file (currently LMPBE22l.MOD) to CALGRID. This file contains the details of the chemical mechanism, such as; the species included, the specific reactions, the rate constants, photolysis data, and the hydrocarbon lumping. This file also contains the number and names of species which are to be treated as transported species or pseudo steady-state species.

Carter's mechanism software also produces the mechanism specific subrou-

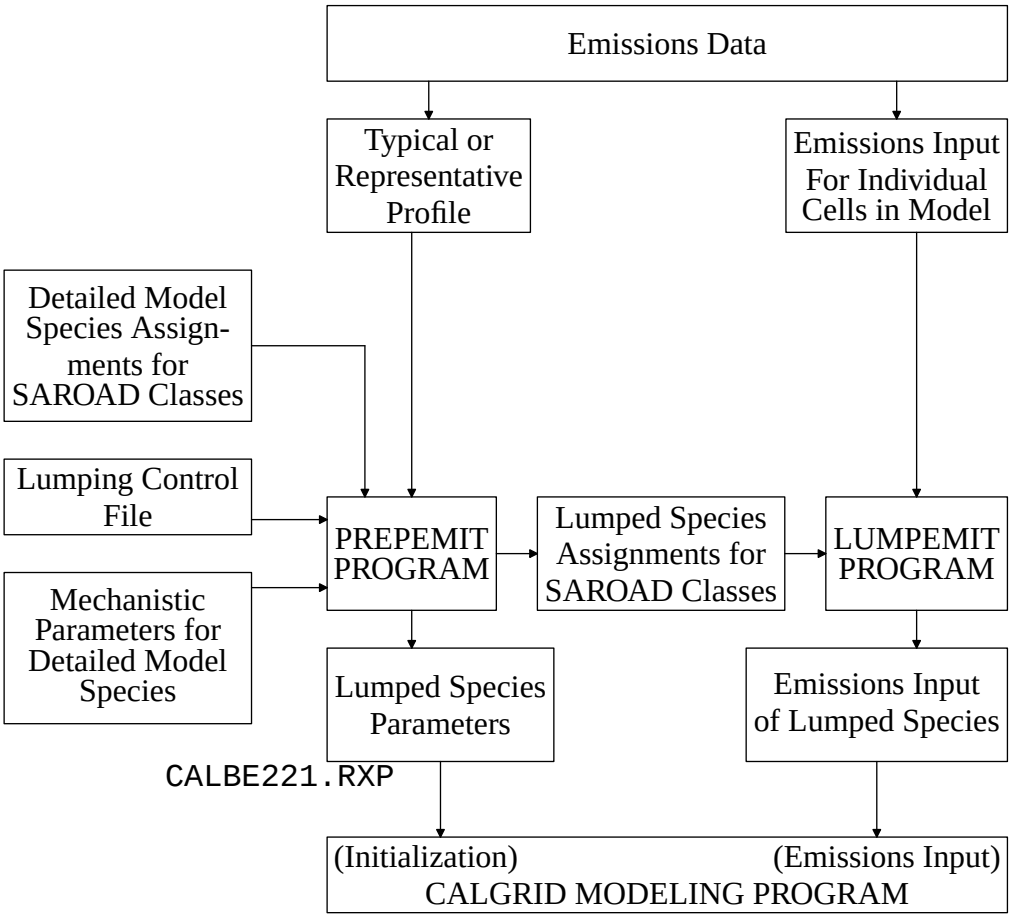

Figure 2.7-1: Overview of the relationships between data files and programs used in the emissions processing system.

tines named CONSTR, DIFUN, and BLDUP which are used in the CALGRID model to formulate the equations used in the chemical integration. Thus, to change the chemical mechanism, the two input files and the three mechanism specific subroutines must be updated. Carter (1988) also has prepared software to easily generate the input files. The relationship of Carter's FORTRAN subroutine and chemical mechanism generation software to the CALGRID program is depicted in Figure 2.7-2.

In addition to these changes, a modification of the chemical mechanism would require that the master species list (the CSPEC array) in block data be updated to reflect the new species names. The quality assurance checks in subroutine INPQA, which verify that the user's control file inputs NSPEC (total number of steady-state plus advected species) and NSA (number of advected species) are consistent with the LMPBE221 mechanism would also have to be modified. The chemistry input file names (LMPBE221.MOD and CALBE221.RXP) opened in subroutine CHEMI should be modified to reflect the new mechanism name.

The parameter file, PARAMS.GRD, contains a variable (MXSPEC) which sets the maximum number of total species to 47. If the number of species is increased beyond 47, this parameter would have to be modified. In addition, if more species are added, modification may be necessary to subroutines which call the control file reader (READIN). This is due to the requirement that each species be included as a call argument to the READIN routine. Appendix A contains a list of all the subroutines which call READIN. It should also be noted that the current limitation of the number of variables in a single input group is 60. Increasing this limit would require modification of subroutine READIN.

Although CALGRID was designed to make changing the chemical mechanism relatively easy, such a change should not be attempted without a thorough understanding of the current structure of the code.

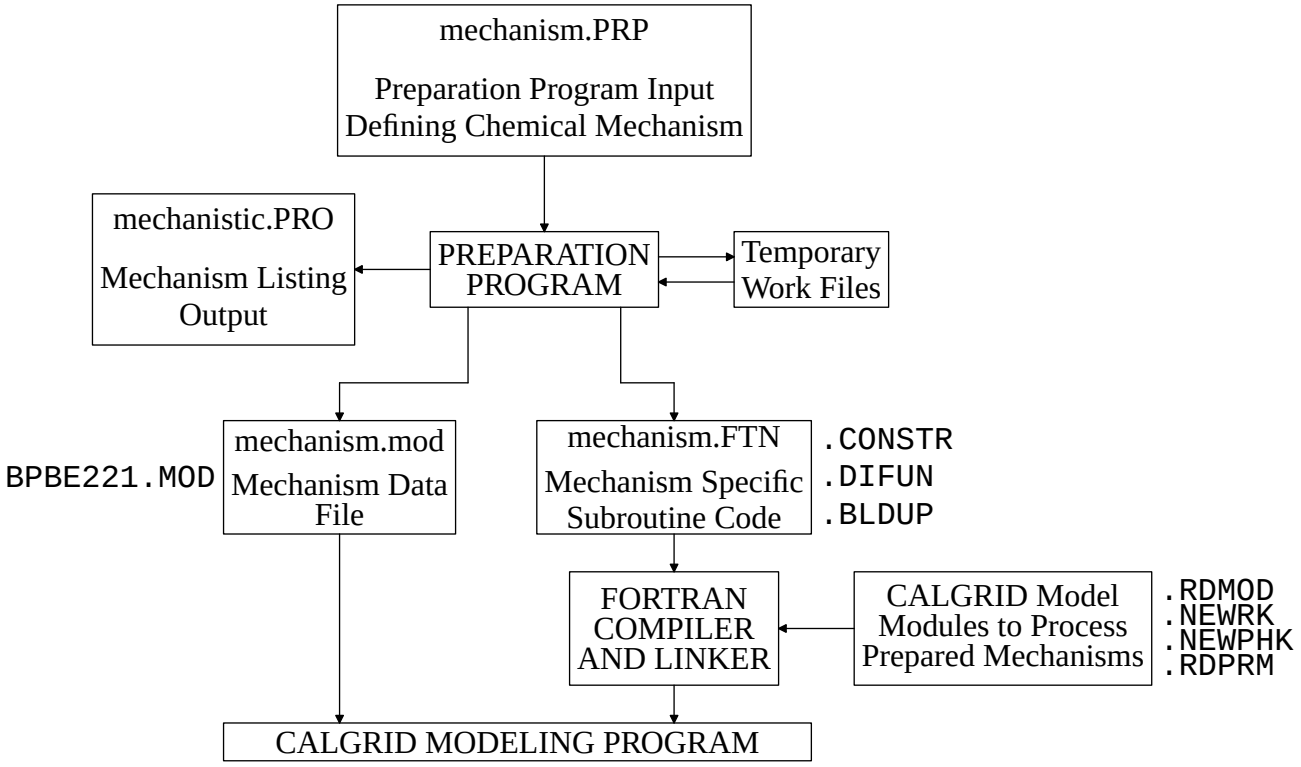

Figure 2.7-2: Overview of the relationships between data files and programs used in the preparation of chemical mechanisms for CALGRID calculations.

3 MODEL STRUCTURE

3.1 Memory Management

A flexible internal memory management scheme is used in CALGRID which eliminates the restriction on certain model parameters arising out of the need to pre-specify array dimensions. Arrays dealing with the number of horizontal grid cells are dynamically allocated by internally partitioning a simple "master" array. The model's main concentration. flux. emissions, meteorological, and work arrays are internally sized and partitioned within the master array. This partitioning is performed automatically in the setup phase of each run to meet its specific storage requirements. The size of individual1 arrays is flexible, subject to the requirement that the total requested storage of all arrays not exceed the size of the master array and individual maximum size parameters in the control file.

The subarrays within the master array are shown in Table 3.1-1. The storage requirement of each subarray is shown in Table 3.1-2 for a 20×20 grid, 10 vertical layers, 36 advected species, and 13 emitted species. The required storage of the subarrays stored in the master array for the example are 359,080 words of which approximately 40% is used for the 4-D concentration array.

In the setup phase of each run, the model prints a table showing the name, dimensions, length, starting and ending addresses of each subarray within the master array. If enough space is not allocated for the master array, the program terminates with an error message requesting that more space be allocated. The use of the master array increases the flexibility of the code, and allows memory to be used efficiently. The master array can easily be adapted to exactly meet the program's needs for a particular application. The internal partitioning relieves the user of the necessity of redimensioning individual arrays and work buffers when the new parameters are modified.

Most of the model's arrays that are not part of the master array are dimensioned with parameter statements. Typically. these arrays are much smaller than the arrays contained within the master array and therefore can be overspecified without a significant effect on the memory requirements of the model. The parameter statements are stored in a file called '`PARAMS.GRD`'. The parameter names and definitions are listed in Table 3.1-3. This file

Table 3.1-1
Subarrays Within The Master Array

No.	Array Name	Dimension	Description
		Concentration Arrays	
1	FULCON	(NX,NY,NZ,NSA)	Main concentration array (ppm)
2	CONAVG	(NX,NY,NSZAVG)	Time averaging array for concentrations (ppm) printed or stored in the output file
3	COLCON	(NSA,NZ)	Concentration array (ppm) holding one vertical column of grid cells used in the central operator
4	TOPCON	(NSA,NX,NY)	Top boundary conditions (ppm)
		Meteorological Variables - Met. Grid	
5	UMET	(NXM, NYM, NZM)	U component of winds (m/s)
6	VMET	(NXM, NYM, NZM)	V component of winds (m/s)
7	WMET	(NXM, NYM, NZM)	W component of winds (m/s) (Note: W defined at grid faces starting at top of cell #1)
8	VMET	(NXM, NYM, NZM)	Air temperature (deg. K)
9	HTMIX	(NXM, NYM)	PGT stability class
10	HTMIX	(NXM, NYM)	Mixing height (m)
11	USTAR	(NXM, NYM)	Friction velocity (m/s)
12	XMONIN	(NXM, NYM)	Monin-Obukhov length (m)
13	WSTAR	(NXM, NYM)	Convective velocity scale (m/s)
		Meteorological Variables - Model Grid	
14	UGRID	(NX, NY, NZ)	U component of winds (m/s) interpolated to CALGRID model layers
15	VGRID	(NX, NY, NZ)	V component of winds (m/s) interpolated to CALGRID model layers
16	WGRID	(NZ+1, NX, NY)	W component of winds (m/s) interpolated to CALGRID model layers
17	TGRID	(NX, NY, NZ)	Air temperature (deg. K) interpolated to model layers
18	PGRID	(NX, NY, NZ)	Pressure (m/s) at each grid point
19	DIFFKH	(NX, NY, NZ)	Lateral diffusivity (m^2/s)

Table 3.1-1
Subarrays Within The Master Array

No.	Array Name	Dimension	Description
20	DIFFKZ	(NZ+1, NX, NY)	Vertical diffusivity (m^2/s) at each cell face
		Geophysical Variables	
21	ZO	(NX, NY)	Surface roughness length (m)
22	ILANDU	(NX, NY)	Land use category (negative values indicate irrigated land)
23	ELEV	(NX, NY)	Terrain elevations (m)
24	XLAI	(NX, NY)	Leaf area index
25	NEARS	(NX, NY)	Nearest surface meteorological station to each grid point
		Emissions - Area & Point Sources	
26	EMAREA	(NX,NY,NSE)	Area source emissions (g/s) for each grid column
27	EMTOT	(NX,NY,NZ,NSE)	Total (area and point source) emission rates
28	EMCOL	(NSA,NZ)	Emissions of a column of grid cells organized for the central operator
29	QAVE	(NSE)	Average emission rates (gis) for a point source in the PTEMCYC file
30	QFDOW	(NWKCAT,NWKADJ)	Day of week emission factors for a point source in the PTEMCYC file
31	SFDOW	(NWKCAT,2)	Day of week stack factors (temp., flow rates) for a point source in the PTEMCYC file
32	QFDI	(NDI, NDIADJ, NDICAT)	Diurnal emission factors for a point source in the PTEMCYC file
33	SFDI	(NDI, 2, NDICAT)	Diurnal stack factors (temp., flow rates) for a point source in the PTEMCYC file
34	TIEM2	(7,NSRC2)	Time invariant stack data for point sources in the PTEMARB file
35	EM2DAT	(NSE2+3,NSRC2)	Time-varying stack and emissions data for point sources in the PTEMARB file

Table 3.1-1
Subarrays Within The Master Array

No.	Array Name	Dimension	Description
36	TIEM3	(8+NSE3,NSRC3)	Time-invariant stack and emissions data for mobile point sources in the PTEMMOB file
37	EM3DAT	(2,NSRC3)	Time varying source coordinates for mobile point sources in the PTEMMOB file
		Dry Deposition and Top Fluxes	
38	VD	(NX, NY, NDIM)	Gridded deposition velocities (m/s) for each deposited pollutant
39	DRYFLX	(NX, NY, NDIM)	Gridded deposition dry fluxes (g/m^2/s) for each deposited pollutant
40	TOPFLX	(NX, NY, NSA)	Top fluxes (g/m^2/s) for each advected species
		Grid Parameters	
41	HTFACE	(NZ+1, NX, NY)	Height (m) of each cell face
42	HTGRID	(NZ, NX, NY)	Height (m) of each grid point
43	DZCELL	(NX, NY)	Array of cell depths (m)
44	XX	(NX)	Array of grid point x coordinates (m)
45	YY	(NY)	Array of grid point y coordinates (m)
		Work Arrays	
46	TMP1	(NWORDS)	Work array
47	TMP2	(NWORDS)	Work array
48	BC	(NZ, MXBTYP, NSA)	Boundary type for each boundary cell
49	ADV1	(NSA, NZ,MAXXY, 4)	Work array
50	ADV2	(NSA, MAX3D)	Work array
51	ADV3	(NSA, MAXXY,4)	Work array

Definition of Variables Used Array Dimension

NX	Number of CALGRID grid cells in the x direction
NY	Number of CALGRID grid cells in the y direction
NZ	Number of vertical layers
NSA	Number of advected species

NXM	Number of x grid cells in the meteorological input file
NYM	Number of y grid cells In the meteorological input file
NZM	Number of z grid cells in the meteorological input file
NSE	Number of emitted species
NWKCAT	Number of day of week categories
NWKADJ	Number of species groups in each day of week category
NDICAT	Number of diurnal adjustment categories per week
NDIADJ	Number of species groups in each diurnal adjustment category
NDI	Number of diurnal adjustment factors in each day
NSRC2	Number of point sources with arbitrarily-varying emission in the PTEMARB data file
NSE2	Number of emitted species in the PTEMARB data file
NSRC3	Number of mobile point sources in the PTEMARB data file
NSE3	Number of emitted species in the PTEMMOB data file

Derived Variables

NSZAVG	Number of species-layer combinations time-averaged for output purposes
NDIM	Maximum of (NSDD,1)
NWORDS	Maximum of (NX+NY,NZ+MXSPEC, (NZ+1)(NZ), (NZM+1)(NZ), 2+NX+2(NY-2))
MAXXY	Maximum of (NX,NY)
MAX3D	Maximum of (WX,NY,NZ)

Table 3.1-2

Sample Partitioning of the Master Array 1nto Subarrays
For a Run With a 20 x 20 Grid, 10 Vertical Layers,
36 Advected Species, and 13 Emitted Species

SUMMARY TABLE OF SUBARRAYS CONTAINED WITHIN THE MASTER ARRAY

Master array size: 375000 (words)
Used in current run: 359080 (words)

Number	Name	Array Dimensions				Array Size (words)	Beg. Address	End Address
1	FULCON	20	20	10	36	144000	01	144000
2	CONAVG	20	20	54	1	21600	144001	165600
3	COLCON	36	10	1	1	360	165601	165960
4	TOPCON	36	20	20	1	14400	165961	180360
5	UMET	20	20	10	1	4000	180361	184360
6	VMET	20	20	10	1	4000	184361	188360

Table 3.1-2

Sample Partitioning of the Master Array 1nto Subarrays
For a Run With a 20 x 20 Grid, 10 Vertical Layers,
36 Advected Species, and 13 Emitted Species

SUMMARY TABLE OF SUBARRAYS CONTAINED WITHIN THE MASTER ARRAY

Master array size: 375000 (words)
Used in current run: 359080 (words)

Number	Name	Array Dimensions				Array Size (words)	Beg. Address	End Address
7	WNET	20	20	10	1	4000	188361	192360
8	TMET	20	20	10	1	4000	192361	196360
9	IPGT	20	20	1	1	400	196361	196760
10	HTMIX	20	20	1	1	400	196761	197160
11	USTAR	20	20	1	1	400	197161	197560
12	XMONIN	20	20	1	1	400	197561	197960
13	WSTAR	20	20	1	1	400	197961	198360
14	UGRID	20	20	10	1	4000	198361	202360
15	VGRID	20	20	10	1	4000	202361	206360
16	WGRID	11	20	20	1	4400	206361	210760
17	TGRID	20	20	10	1	4000	210761	214760
18	PGRID	20	20	10	1	4000	214761	218760
19	DIFFKH	20	20	10	1	4000	218761	222760
20	DIFFKZ	11	20	20	1	4400	222761	227160
21	Z0	20	20	1	1	400	227161	227560
22	ILANDU	20	20	1	1	400	227561	227960
23	ELEV	20	20	1	1	400	227961	228360
24	XLAI	20	20	1	1	400	228361	228760
25	NEARS	20	20	1	1	400	228761	229160
26	EMAREA	20	20	13	1	5200	229161	234360
27	EMTOT	20	20	10	13	52000	234361	286360
28	EMCOL	36	10	1	1	360	286361	286720
29	QAVE	13	1	1	1	13	286721	286733
30	QFDOW	1	1	1	1	1	286734	286734
31	SFDOW	1	2	1	1	2	286735	286736
32	QFDI	1	1	1	1	1	286737	286737
33	SFDI	1	2	1	1	2	286738	286739
34	TIEM2	7	3	1	1	21	286740	286760
35	EM2DAT	16	3	1	1	48	286761	286808
36	TIEM3	21	4	1	1	84	286809	286892
37	EM3DAT	2	4	1	1	8	286893	286900
38	VD	1	20	15	1	6000	286901	292900
39	DRYFLX	20	20	15	1	6000	292901	298900
40	TOPFLX	20	20	36	1	14400	298901	313300
41	HTFACE	11	20	20	1	4400	313301	317700
42	HTGRID	10	20	20	1	4000	317701	321700

Table 3.1-2

Sample Partitioning of the Master Array 1nto Subarrays
For a Run With a 20 x 20 Grid, 10 Vertical Layers,
36 Advected Species, and 13 Emitted Species

SUMMARY TABLE OF SUBARRAYS CONTAINED WITHIN THE MASTER ARRAY

Master array size: 375000 (words)
Used in current run: 359080 (words)

Number	Name	Array Dimensions				Array Size (words)	Beg. Address	End Address
43	DZCELL	20	20	1	1	400	321701	322100
44	XX	20	1	1	1	20	322101	322120
45	YY	20	1	1	1	20	322121	322140
46	TMP1	470	1	1	1	470	322141	322610
47	TMP2	470	1	1	1	470	322611	323080
48	BC	10	10	36	1	3600	323081	326680
49	ADV1	36	10	20	4	28800	326681	355480
50	ADV2	36	20	1	1	720	355481	356200
51	ADV3	36	20	4	1	2880	356201	359080

is inserted into any CALGRID subroutine requiring a parameter via the Fortran 'include' statements. Thus, a global redimensioning of cell variables using any of these parameters can be accomplished simply by modifying the PARAMS.GRD file and recompiling the program.

Table 3.1-3
Sample CALGRID Parameter File

```
c-----------------------------------------------------------------------
c --- PARAMETER statements                                        CALGRID
c-----------------------------------------------------------------------
c
c --- Specify parameters
      parameter(mxmain=375000,mxarr=51)
      parameter(mxspec=47)
      parameter(mxnxy=20,mxnz=10)
      parameter(mxnzm=25,mxss=50)
      parameter(mxpdep=1,mxint=9)
      parameter(mxbtyp=10)
      parameter(mxsg=8,mxvar=60,mxcol=132)
      parameter(io5=1,io6=2,io7=7,io8=8,io9=9,io10=10,io11=11,io12=12)
      parameter(io15=15,io16=16,io17=17,io18=18,io20=20)
c
c --- Compute derived parameters
      parameter(mx2=2*mxspec,mx4=4*mxspec,mx5=5*mxspec,mxnzp1=mxnz+1)
      parameter(mxnsnz=mxspec*mxnz)
      parameter[mxnzmp1=mxnzm+1)
      parameter(mxiop=2*mxnz+2)
c
c --- GENERAL PARAMETER definitions:
c        MXMAIN - Dimension of master array
c         MXARR - Maximum number of subarrays into which the master
c                 array can be partitioned
c        MXSPEC - Maximum total number of chemical species (advected +
c                 steady-state species)
c         MXNXY - Maximum number of cells in the X or Y directions
c                 (MXNXY must be greater than or equal to the greater
c                 of NX and NY)
c          MXNZ - Maximum number of vertical layers allowed
c         MXNZM - Maximum number of vertical layers in input CALMET
```

```
c                 meteorological data fields
c          MXSS - Maximum number of surface meteorological stations
c                 in the CALMET data
c        MXPDEP - Maximum number of particle species dry deposited
c         MXINT - Maximum number of particle size intervals used
c                 in defining mass-weighted deposition velocities
c        MXBTYP - Maximum number of lateral boundary types (each
c                 boundary type is assigned a species & height dependent
c                 profile of boundary conditions)
c
c --- CONTROL FILE READER definitions:
c          MXSG - Maximum number of input groups in control file
c         MXVAR - Maximum number of variables in each input group
c         MXCOL - Maximum length (bytes) of a control file input record
c
c --- FORTRAN I/O unit numbers:
c            IO5 - Control file (CALGRID.INP)    - input  - formatted
c            IO6 - List file (CALGRID.LST)       - output - formatted
c
c            IO7 - Meteorological data file      - input  - unformatted
c                  (CALMET.DAT)
c
c            IO8 - Concentration output file     - output - unformatted
c                  (CONC. DAT )
c            IO9 - Dry flux output file          - output - unformatted
c                  (DFLX.DAT)
c
c           IO10 - Initial concentration file    - input  - formatted or
c                  (ICON.DAT)                              unformatted
c           IO11 - Lateral boundary condition    - input  - formatted or
c                  file (BCON.DAT)                         unformatted
c           IO12 - Top boundary condition file   - input  - formatted or
c                  (TCON.DAT)                              unformatted
c
c           IO15 - Pt. source emissions file #1   - input - unformatted,
c                  (PTEMCYC.DAT) - Cyclical or             DIRECT-ACCESS
c                  constant emission parameters
c           IO16 - Pt. source emissions file #2   - input - unformatted
c                  (PTEMARB.DAT) - Arbitrarily-
c                  varying point source emissions
```

```
c           IO17 - Pt. source emissions file #3   - input - unformatted
c                  (PTEMMOB.DAT) - Mobile point
c                  source emissions
c           IO18 - Area source emissions          - input - unformatted
c                  (AREM.DAT)
c           IO20 - User-specified deposition      - input - formatted
c                  velocities (VD.DAT)
c
c           NOTE:  Units 31 (LMPBE22l.MOD),
c                        32 (CALBE22l.RXP), and
c                        33 (CHMOUT1)
c                  are reserved for use by the chemistry module
c
```

3.2 Structure of the CALGRID Driver Program and Major Modules

The CALGRID model execution is divided into three major phases: setup, computational, and termination (see Figure 3.2-1). In the setup phase of the model execution, a variety of initialization and one-time I/O and computational operations are performed, including the following:

- Opening of input and output files.
- Reading and processing the control file inputs which includes model option flags and run control variables.
- Memory management operations such as the partitioning of the master array.
- Reading and processing the header records or data files of the model's input data bases (emissions files, meteorological data file, initial and boundary condition files, and chemistry files).
- Performing consistency checks of the input data base information versus the control file inputs
- Computing various cross-referencing arrays required to interface data in the model input files with the model subroutines.
- Performing initialization and setup operations for the horizontal and vertical advection/diffusion operators, dry deposition module, and chemistry module.

- Writing the header records to the model's output concentration and dry flux files.

The computational phase of the model includes the basic time loop within which the solution of the governing equation is advanced. The functions performed in the computation phase include the following:

- Retrieving and processing of the emissions, meteorological, and boundary condition data from the appropriate input files
- Computing solutions for equations governing horizontal advection/diffusion, vertical advection/diffusion, dry deposition, and gas phase chemistry.
- Time averaging and output of gridded hourly fields of concentrations and dry fluxes.

The final phase of the model execution deals with run termination functions. The termination phase includes the closing of any active data files, computation of model runtime, and printing of summary or normal termination messages.

A flow diagram for the setup module is provided in figure 3.2-2. The flow diagram contains the name of each subroutine or function called by the setup module along with a brief description of the routine's purpose. A complete listing of the subroutine calling sequence, including second and higher order subroutine/function calls, is provided in Appendix A.

The task of time integration of the equations describing the physical and chemical system is complicated by the range of characteristics and behavior of the various equations. For example, the highly stiff set of nonlinear chemical equations requires specialized numerical treatment. The solution of the horizontal and vertical advection and diffusion equations poses different problems. Therefore, the numerical solution of the system of equations is most efficiently obtained by decomposing the time advancement operator into a number of component operators. This operator splitting (Marchuk, 1975) allows specialized numerical techniques to be applied that are optimized for each of the individual operators. An additional effect of the operator splitting is that overall program flexibility is increased because program modularity is facilitated.

The time development operator in ADOM/TADAP is factorized in the following way:

$$C_{t+\delta t} = L_x L_y L_z L_c L_z L_y L_x C_t$$

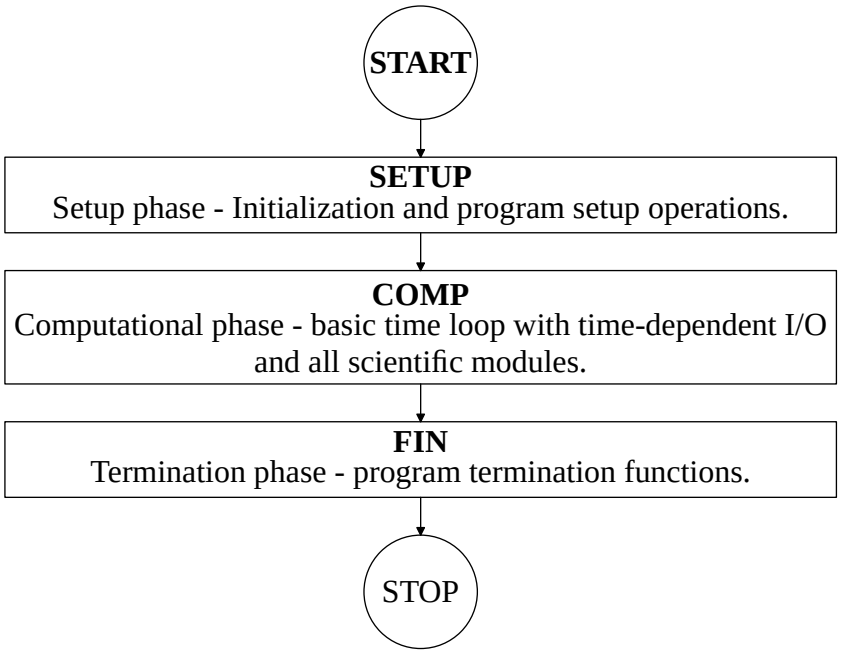

Figure 3.2-1: Flow diagram showing the subroutine calling sequence in the `CALGRID MAIN` program.

where C_t, $C_{t+\delta t}$ are the concentrations at time t and $t + \delta t$,

L_x is the one-dimensional horizontal advection and diffusion operator (x direction),

L_y is the one-dimensional horizontal advection and diffusion operator (y direction),

L_z is the one-dimension operator including vertical advection. diffusion, emissions injection, and dry deposition,

L_c is the "central operator" consisting of the chemical mechanism solver.

Each of these operators, except for the central operator, is applied twice for each basic time step (i.e., time at intervals of $\delta t/2$). The central operator is applied only once each time step over a full time interval of δt.

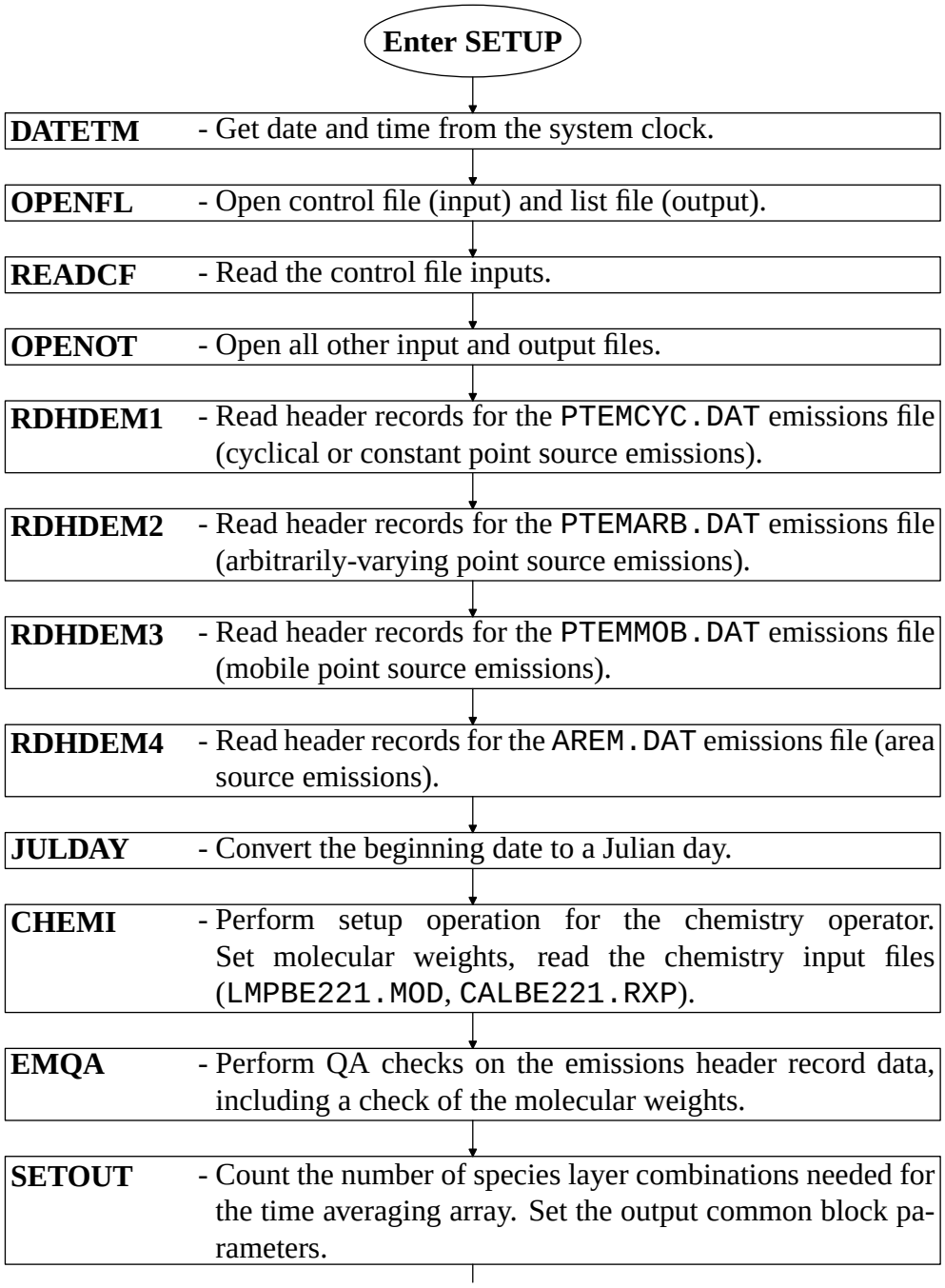

Figure 3.2-2: Flow diagram showing the subroutine/function calling sequence in the subroutine SETUP (setup phase).

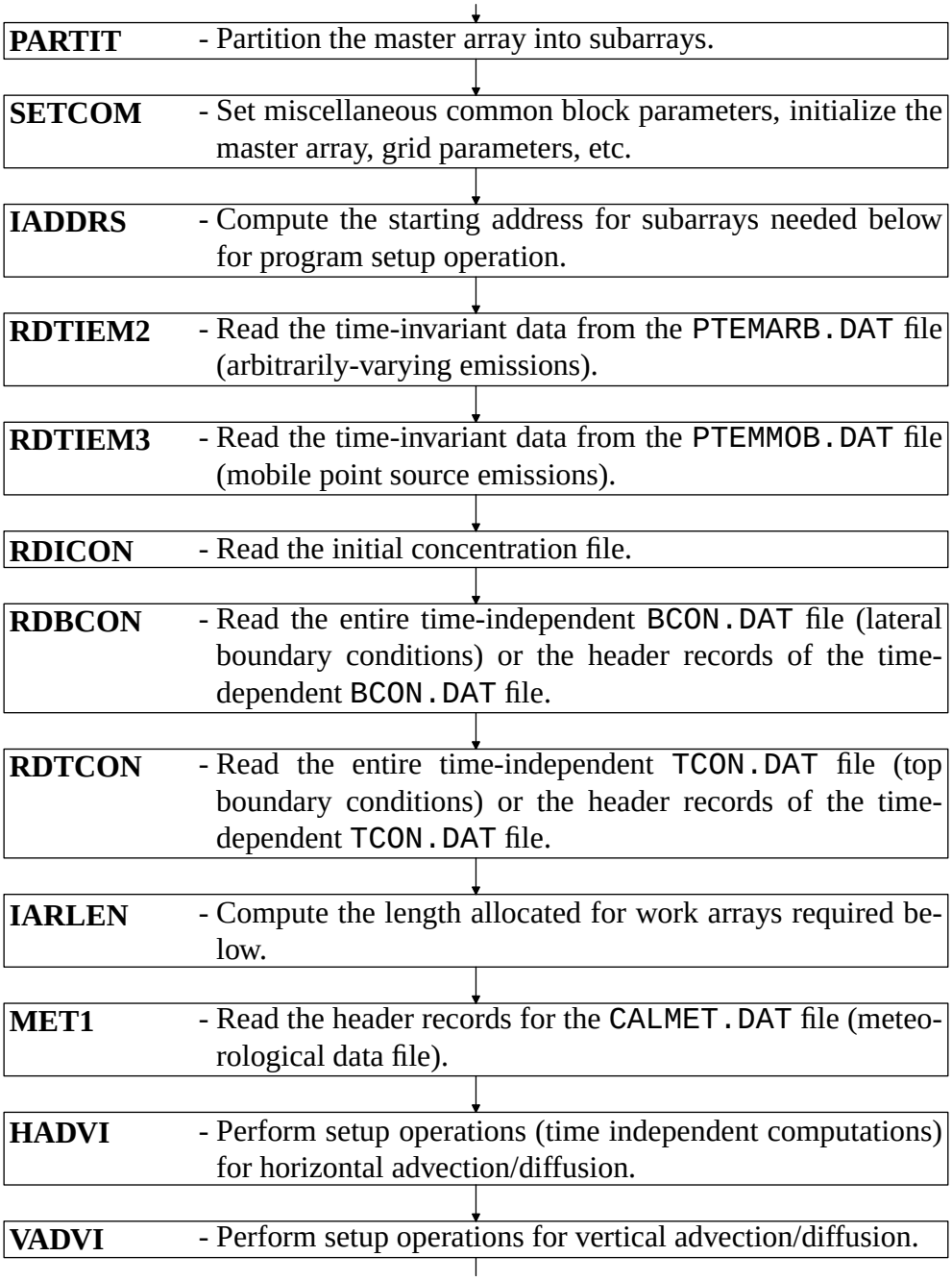

Figure 3.2-2: Flow diagram showing the subroutine/function calling sequence in the subroutine SETUP (setup phase) (continued).

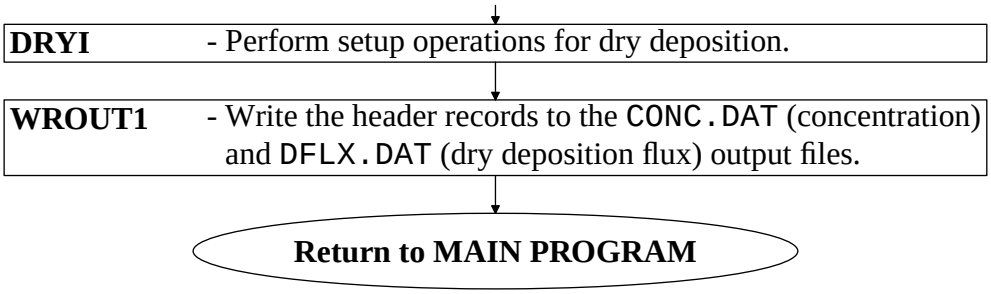

Figure 3.2-2: Flow diagram showing the subroutine/function calling sequence in the subroutine SETUP (setup phase) (concluded).

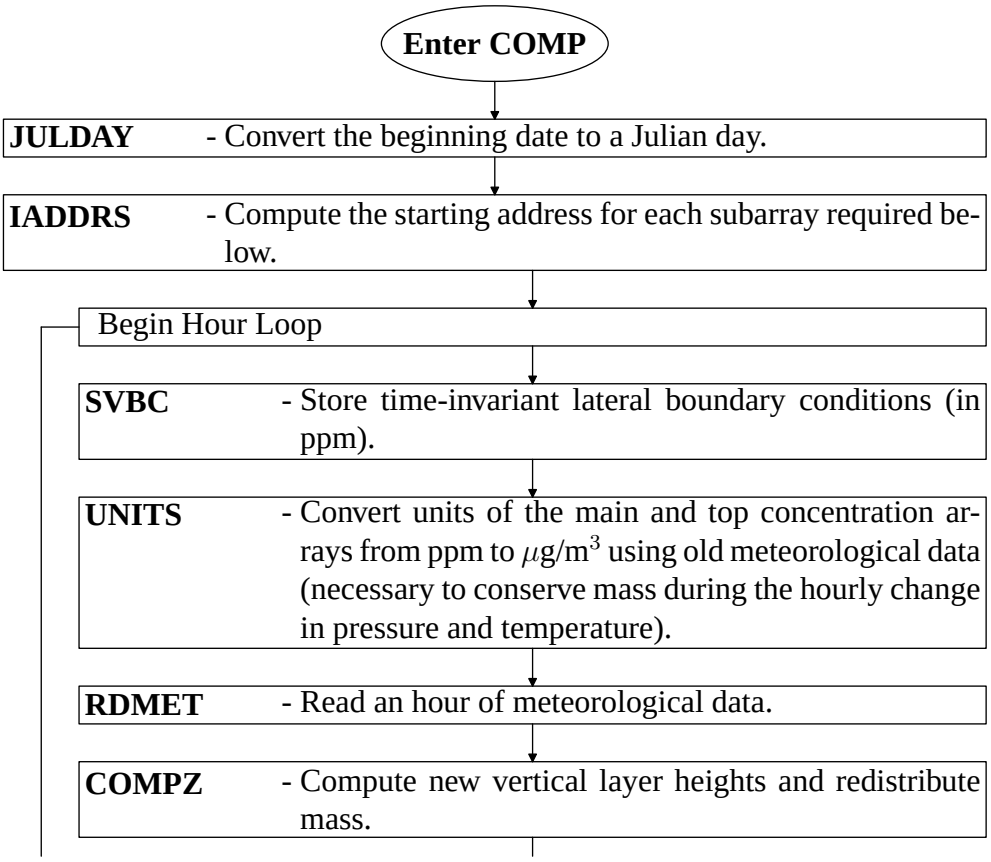

Figure 3.2-3: Flow Diagram showing the subroutine/function calling sequence in subroutine COMP (Computational Phase).

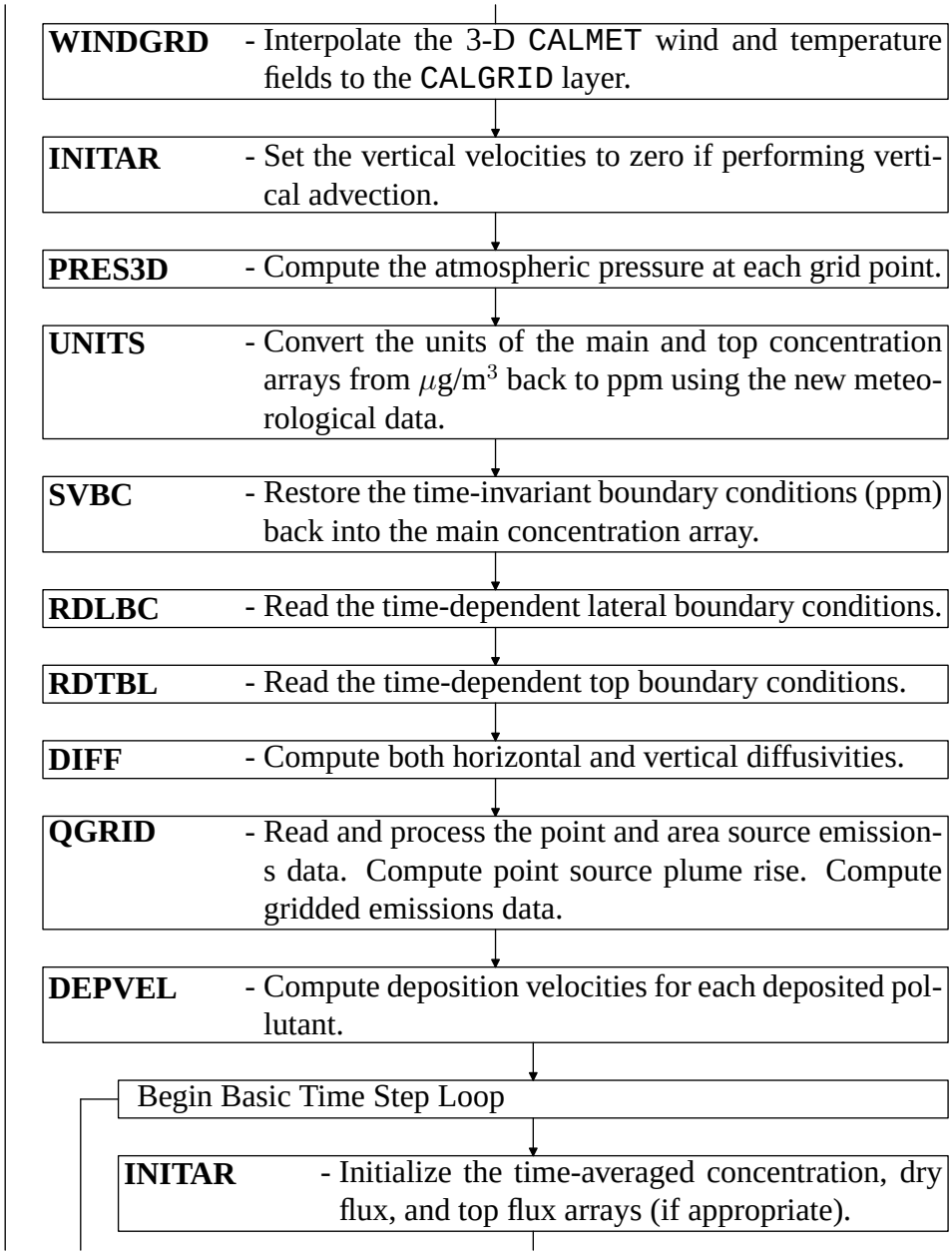

Figure 3.2-3: Flow Diagram showing the subroutine/function calling sequence in subroutine COMP (Computational Phase) (continued).

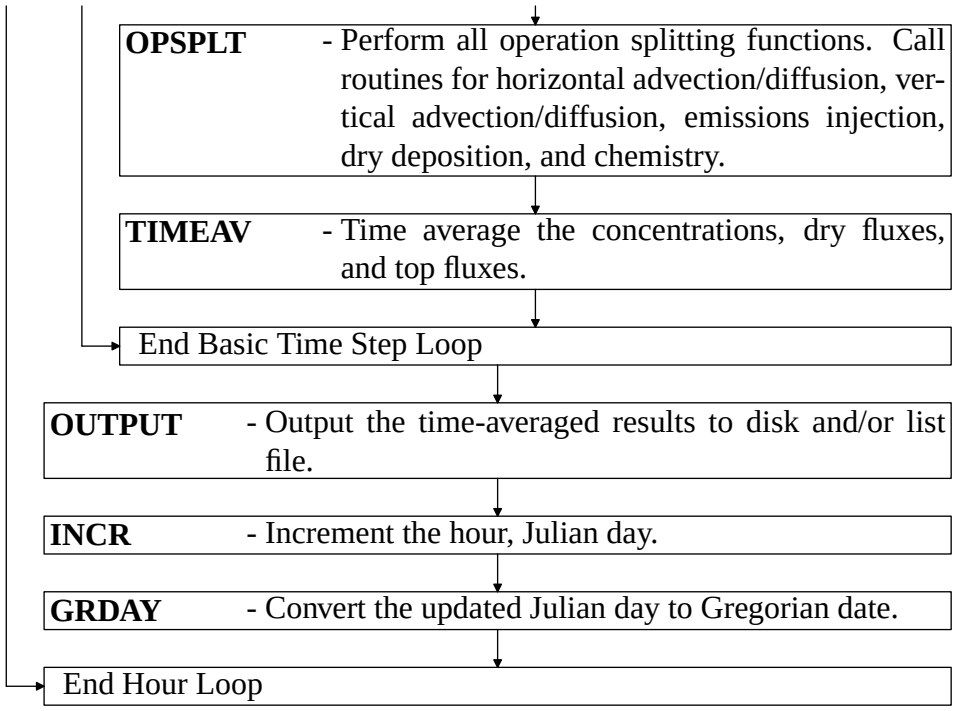

Figure 3.2-3: Flow Diagram showing the subroutine/function calling sequence in subroutine `COMP` (Computational Phase) (concluded).

4 DATA BASE CONTENTS AND FORMATS

4.1 Input Files

4.1.1 User Control File (CALGRID.INP)

The selection and control of CALGRID options are determined by user-specified inputs contained in a file called the control file This file, CALGRID.INP, contains all the information necessary to define a model run (e.g., starting date, run length, grid specifications, technical options, output options, etc.).

A sample control file is shown in Figure 4.1.1. It is designed to be flexible and easy-to-use. The control file is read by a set of Fortran text processing routines contained within CALGRID which allow the user considerable flexibility in designing and customizing the input file. An unlimited amount of optional descriptive text can be inserted within the control file to make it self-documenting. For example, the definition, allowed values, units, and default value of each input variable can be included within the control file.

The control file processor searches for pairs of special delimiter characters (!). All text outside the delimiters is assumed to be user comment information and is echoed back but otherwise ignored by the input module. Only data within the delimiter characters is processed. The input data consists of a leading delimiter followed by the variable name, equals sign, input value or values, and a terminating delimiter (e.g., !XX = 12.5!). The variable name can be lower or upper case, or a mixture of both (i.e., XX, xx, Xx are all equivalent). The variable can be a real, integer or logical array or scalar. The use of repetition factors for arrays is allowed (e.g., ! XARRAY = 3 * 1.5 ! instead of XARRAY = 1.5, 1.5, 1.5 !). Different values must be separated by commas. Spaces within the delimiter pair are ignored. Exponential notation (E format) for real numbers is allowed. However, the optional plus sign should be omitted (e.g., enter +1.5E+10 as 1.5E10). The data may be extended over more than one line. The line being continued must end with a comma. Each leading,delimiter must be paired with a terminating delimiter. All text between the delimiters is

```
TEST RUN ppm version --  5 hours starting at 08:00 PST, 7/01/80
10 Fixed Layers -- Horizontal grid -- 20 x 20
Time step = 1/3 hour
---------------- Run title (3 lines) ----------------------------------------


                       CALGRID MODEL CONTROL FILE

Additional user comments
------------------------


Uses test point and area source emissions (PTEMCYC, PTEMARB, PTEMMOB, AREM)

Uses formatted initial concentration file, boundary condition file, and
top boundary condition file

Uses user-supplied deposition velocities for HNO3 and SO2

--------------------------------------------------------------------------------

INPUT GROUP: 1 -- General run control parameters
--------------

     Starting date:   Year (IBYR) -- No default       ! IBYR=80 !
                     Month (IBMO) -- No default       ! IBMO=7  !
                       Day (IBDY) -- No default       ! IBDY=1  !
                      Hour (IBHR) -- No default       ! IBHR=8  !

     Length of run (hours) (IRLG) -- No default       ! IRLG=5 !

     Number of time steps
     per hour (NSUBTS)            -- Default: 3       ! NSUBTS= 3 !
     (Time step (sec) = 3600./NSUBTS)

     Total number of chemical species
     (advected + steady-state species) (NSPEC)
                                     Default: 47      ! NSPEC=47 !

     Number of chemical species
     to be advected (NSA)            Default: 36      ! NSA=36  !

     Number of chemical species
     to be deposited (NSDD)          Default: 15      ! NSDD=15 !

     Number of chemical species
     to be emitted  (NSE)            Default: 13      ! NSE=13 !

     Method flag for integration of
     chemical mechanism (METHINT)    Default: 2       ! METHINT=2 !
         1 = Hybrid method
         2 = QSSA method


     INPUT FILE TYPES:
```

```
Initial Concentration (ICON.DAT) file
-------------------------------------

                           Default: 1      ! ITICON=1 !

  ITICON = 1 for a formatted text file containing one
             concentration value per layer per species
  ITICON = 2 for an unformatted file containing a full
             3-D set of concentrations for each species
             (NX * NY * NZ * NSA values)

Side Boundary Concentration (BCON.DAT) file
-------------------------------------------

                           Default: 1      ! ITBCON=1 !

  ITBCON = 1 for a formatted text file containing boundary
             types and time-independent boundary conditions
             as a function of height for each advected species
  ITBCON = 2 for an unformatted file containing a full
             set of boundary conditions for each advected species
  ITBCON = 3 if BCON file is not used.  Time-independent
             boundary conditions are taken from the initial
             concentration file.


Top Boundary Concentration (TCON.DAT) file
------------------------------------------

                           Default: 1      ! ITTCON=1 !

  ITTCON = 1 for a formatted text file containing time-independent
             top boundary conditions for each advected species.
  ITTCON = 2 for an unformatted file containing an full
             set of time- and space-dependent top boundary
             conditions for each advected species.
  ITTCON = 3 if TCON file is not used.  The top layer of the
             initial concentration distribution is used to obtain
             time-independent top boundary conditions.


Stationary Point Source Emissions File with cyclical
or constant emissions (PTEMCYC.DAT)
-----------------------------------------------------

                           Default: 1      ! ITEM1=1 !

  ITEM1  = 1 if the unformatted, direct-access PTEMCYC input
             file is used.
  ITEM1  = 2 if the PTEMCYC file is not used.


Stationary Point Source Emissions File with arbitrarily
varying emissions (PTEMARB.DAT)
-------------------------------------------------------
```

```
                              Default: 1      ! ITEM2=1 !

  ITEM2  = 1 if the unformatted PTEMARB input file is
             used.
  ITEM2  = 2 if the PTEMARB file is not used.


Mobile Point Source Emissions File (PTEMMOB.DAT)
(constant emissions)
------------------------------------------------

                              Default: 1      ! ITEM3=1 !

  ITEM3  = 1 if the unformatted PTEMMOB input file is
             used.
  ITEM3  = 2 if the PTEMMOB file is not used.


Area Source Emissions File (AREM.DAT)
-------------------------------------

                              Default: 1      ! ITEM4=1 !

  ITEM4  = 1 if the unformatted AREM input file is
             used.
  ITEM4  = 2 if the AREM file is not used.


Distribution Function for Area Source Emissions
-----------------------------------------------
Area source emissions can be distributed among
several layers according user-specified weighting
factors

   - Fraction of mass distributed into each
     user-defined "emissions" layer (WTEM(nzem))
     Defaults:  0.75, 0.25                     ! WTEM = 0.75, 0.25 !
     NOTE: NZEM values must be entered and must
           add up to 1.0

   - Number of emissions layers (NZEM)
     Default: 2                                ! NZEM = 2 !
     NOTE: Up to MXNZ layers are allowed, where
           MXNZ is defined in the parameter file

   - Height (m) of each emission layer face
     (ZFEM(nzem+1))   Default: 0.0, 50., 100.   ! ZFEM = 0., 50., 100. !
     NOTE: NZEM+1 values must be entered.

   (Default values distribute 75% of area source mass
    below 50. m, and 25% between 50-100 m.)


                                              ! IEM1REC=156 !

!END!
```

```
------------------------------------------------------------------------------

INPUT GROUP: 2 -- Grid control parameters
--------------

     Horizontal grid definition:

           No. X grid cells (NX)    No default      ! NX=20 !
           No. Y grid cells (NY)    No default      ! NY=20 !

     Grid spacing (DGRIDKM) (km)       No default      ! DGRIDKM=4.0 !

     Reference UTM coordinates (km)
     of SOUTHWEST corner of grid point (1,1)

        X coordinate (XORIGKM)       No default    ! XORIGKM= 168.000 !
        Y coordinate (YORIGKM)       No default    ! YORIGKM=3839.000 !

            UTM zone (IUTMZN)        No default      ! IUTMZN= 11 !

     Reference coordinates of CENTER
     of the domain (used in the
     calculation of solar elevation angles)

        Latitude  (deg.) (XLAT)      No default    ! XLAT  =  34.0  !
        Longitude (deg.) (XLONG)     No default    ! XLONG = 118.0  !
        Time zone        (XTZ)       No default    ! XTZ   =   8.   !
        (PST=8, MST=7, CST=6, EST=5)

     Vertical grid definition:

        No. of vertical layers in the
        CALMET meteorological grid (NZM)  No default      ! NZM =10 !

        Vertical CALGRID grid type (IVGTYP)  Default: 2   ! IVGTYP=2 !
           IVGTYP = 0 uniform thickness above and
                      below DIFFBREAK
           IVGTYP = 1 dynamically varying layers
           IVGTYP = 2 for arbitrary fixed grid

           Enter values for the following variables based on IVGTYP
              IVGTYP         REQUIRED VARIABLES
              ------         ------------------
                0            NZ, NZL, ZMINB, ZMAXB, ZMINA, ZMAXA, ZTOP
                1            NZ, NZL, DZMIN, ZTOP
                2            NZ, ZFACE(nz+1)
IVGTYP
------
0,1,2    NZ   -- No. of vertical layers        No default      ! NZ =10 !
0,1      NZL  -- No. layers below DIFFBREAK    No default      * NZL = 6     *
0        ZMINB-- Minimum depth (m) of cells    Default: 20.    * ZMINB=20.   *
                 below DIFFBREAK & above layer #1
0        ZMAXB-- Maximum depth (m) of cells    Default: 5000.  * ZMINB=5000. *
```

```
                below DIFFBREAK & above layer #1
0       ZMINA-- Minimum depth (m) of cells    Default: 20.    * ZMINA=20.   *
                above DIFFBREAK
0       ZMAXA-- Maximum depth (m) of cells    Default: 5000.  * ZMINA=5000. *
                above DIFFBREAK
0,1     ZTOP -- Top of domain (m)             No default      * ZTOP =5000. *
  1     DZMIN-- Minimum cell depth (m) for    Default: 20.    * DZMIN=30.   *
                layers above layer #1
    2   ZFACE(nz+1)-- Cell face heights (m)   No defaults
                in arbitrary vertical grid
                                                        ! ZFACE = 0.0, 20.0,
                    80., 160., 260., 410., 660., 1200., 2200., 3600., 5000. !

!END!

-------------------------------------------------------------------------------

INPUT GROUP: 3 -- Species list
--------------

                                                                      DRY
SPECIES        MODELED          ADVECTED          EMITTED          DEPOSITED
 NAME       (0=NO, 1=YES)    (0=NO, 1=YES)   (0=NO, 1=YES)  (0=NO,
                                                                  1=COMPUTED-GAS
                                                                  2=COMPUTED-PARTICLE
                                                                  3=USER-SPECIFIED)

BUILD-UP SPECIES

! CO2          =   1       ,       1       ,      0       ,      0      !
! HO2H         =   1       ,       1       ,      0       ,      1      !
! RO2-HO2-PROD =   1       ,       1       ,      0       ,      0      !
! RO2-RO2-PROD =   1       ,       1       ,      0       ,      0      !
! -OOH         =   1       ,       1       ,      0       ,      1      !
! -C           =   1       ,       1       ,      0       ,      0      !
! -N           =   1       ,       1       ,      0       ,      0      !
! H2           =   1       ,       1       ,      0       ,      0      !
! H2SO4        =   1       ,       1       ,      0       ,      2      !

ACTIVE SPECIES

! O3           =   1       ,       1       ,      0       ,      1      !
! NO           =   1       ,       1       ,      1       ,      0      !
! NO2          =   1       ,       1       ,      1       ,      0      !
! NO3          =   1       ,       1       ,      0       ,      0      !
! N2O5         =   1       ,       1       ,      0       ,      0      !
! HNO3         =   1       ,       1       ,      0       ,      3      !
! HONO         =   1       ,       1       ,      0       ,      1      !
! HNO4         =   1       ,       1       ,      0       ,      1      !
! HO2          =   1       ,       1       ,      0       ,      1      !
! CO           =   1       ,       1       ,      1       ,      0      !
! RO2.         =   1       ,       1       ,      0       ,      1      !
! RCO3.        =   1       ,       1       ,      0       ,      0      !
! PAN          =   1       ,       1       ,      0       ,      1      !
! HCHO         =   1       ,       1       ,      1       ,      1      !
! RNO3         =   1       ,       1       ,      0       ,      1      !
```

```
! MEK          =   1       ,       1       ,      1       ,      0      !
! MGLY         =   1       ,       1       ,      0       ,      0      !
! CRES         =   1       ,       1       ,      0       ,      0      !
! AFG2         =   1       ,       1       ,      0       ,      0      !
! AAR1         =   1       ,       1       ,      1       ,      0      !
! AAR2         =   1       ,       1       ,      1       ,      0      !
! AAR3         =   1       ,       1       ,      1       ,      0      !
! AAR4         =   1       ,       1       ,      1       ,      0      !
! ETHE         =   1       ,       1       ,      1       ,      0      !
! OLE1         =   1       ,       1       ,      1       ,      0      !
! SO2          =   1       ,       1       ,      1       ,      3      !

STEADY-STATE SPECIES

! HO.          =   1       ,       0       ,      0       ,      0      !
! O            =   1       ,       0       ,      0       ,      0      !
! O*1D2        =   1       ,       0       ,      0       ,      0      !
! RO2-R.       =   1       ,       0       ,      0       ,      0      !
! RO2-N.       =   1       ,       0       ,      0       ,      0      !
! R2O2.        =   1       ,       0       ,      0       ,      0      !
! RO2-XN.      =   1       ,       0       ,      0       ,      0      !
! HOCOO.       =   1       ,       0       ,      0       ,      0      !
! -NO2         =   1       ,       0       ,      0       ,      0      !
! O3OL-SB      =   1       ,       0       ,      0       ,      0      !
! H2O          =   1       ,       0       ,      0       ,      0      !
!END!

----------------------------------------------------------------------------
INPUT GROUP: 4 -- Chemical parameters for dry deposition of gases
--------------

SPECIES     DIFFUSIVITY      ALPHA STAR      REACTIVITY    MESOPHYLL RESISTANCE     HENRY'S LAW COEFFICIENT
 NAME        (cm**2/s)                                          (s/cm)                 (dimensionless)
-------     -----------      ----------      ----------    --------------------     ----------------------
! HO2H =      0.2402     ,      1.00     ,      12.0    ,          0.0           ,          4.0e-7         !
! -OOH =      0.1403     ,      1.00     ,      12.0    ,          0.0           ,          1.0e-6         !
! O3   =      0.1594     ,     10.00     ,      15.0    ,          4.0           ,          2.0            !
! NO2  =      0.1656     ,      1.00     ,       8.0    ,          5.0           ,          3.5            !
! NO3  =      0.1656     ,      1.00     ,       8.0    ,          5.0           ,          1.0e-6         !
* HNO3 =      0.1628     ,      1.00     ,      18.0    ,          0.0           ,          8.0e-8         *
! HONO =      0.1100     ,      1.00     ,       4.0    ,          2.0           ,          4.3e-4         !
! HNO4 =      0.1500     ,      1.00     ,       4.0    ,          2.0           ,          1.0e-5         !
! HO2  =      0.2402     ,      1.00     ,      12.0    ,          0.0           ,          1.0e-6         !
! RO2. =      0.2402     ,      1.00     ,      12.0    ,          0.0           ,          1.0e-6         !
! PAN  =      0.1050     ,      1.00     ,       4.0    ,          1.0           ,          1.0e-2         !
! HCHO =      0.2336     ,      1.00     ,       4.0    ,          0.0           ,          4.0e-6         !
! RNO3 =      0.1100     ,      1.00     ,       4.0    ,          2.0           ,          1.0e-6         !
* SO2  =      0.1509     ,      1.00E3   ,       8.0    ,          0.0           ,          4.0e-2         *

!END!

----------------------------------------------------------------------------

INPUT GROUP: 5 -- Size parameters for dry deposition of particles
--------------
       *
```

```
SPECIES      GEOMETRIC MASS MEAN        GEOMETRIC STANDARD
 NAME             DIAMETER                 DEVIATION
                  (microns)                (microns)
-------      ------------------        ------------------
! H2SO4  =          0.48          ,           2.00     !


*
 H2SO4 deposited as sulfate


!END!

------------------------------------------------------------------------------



------------------------------------------------------------------------------

INPUT GROUP: 6 -- Miscellaneous dry deposition parameters
--------------

     Reference cuticle resistance   (RCUTR)  (s/cm)   !  RCUTR=17.0 !
     Reference ground resistance    (RGR)    (s/cm)   !    RGR= 5.0 !
     Reference pollutant reactivity (REACTR)          ! REACTR= 8.0 !

     Vegetation state in unirrigated areas (IVEG)     !   IVEG=1    !
        IVEG=1 for active and unstressed vegetation
        IVEG=2 for active and stressed vegetation
        IVEG=3 for inactive vegetation

!END!



------------------------------------------------------------------------------

INPUT GROUP: 7 -- Output Options
--------------
                                          *                          *
     FILE                        DEFAULT VALUE             VALUE THIS RUN
     ----                        -------------             --------------

   Concentrations (ICON)              1                   !   ICON = 0 !
   Fluxes (IDRY)                      1                   !   IDRY = 0 !

   *
    0 = Do not create file, 1 = create file


    LINE PRINTER OUTPUT OPTIONS:

       Print concentrations (ICPRT)    Default: 0          ! ICPRT = 1 !
       Print dry fluxes (IFPRT)        Default: 0          ! IFPRT = 0 !
       Print top fluxes (ITPRT)        Default: 0          ! ITPRT = 0 !
       Print deposition vel. (IVDPRT)  Default: 0          ! IVDPRT= 0 !
```

```
       (0 = Do not print, 1 = Print)

       No. layers of gridded total
       (area+point) emissions to print
                            (IEPRT)   Default: 0          ! IEPRT= 0 !
       (IEPRT must be <= NZ)


       Concentration print interval
       (ICFRQ) in hours                Default: 1          ! ICFRQ = 1 !
       Dry flux print interval
       (IFFRQ) in hours                Default: 1          ! IFFRQ = 4 !
       Top flux print interval
       (ITFRQ) in hours                Default: 1          ! ITFRQ = 1 !
       Deposition vel. print interval
       (IVDFRQ) in hours               Default: 1          ! IVDFRQ = 4 !
       Emissions print interval
       (IEFRQ) in hours                Default: 1          ! IEFRQ = 4 !
```

SPECIES LIST FOR OUTPUT OPTIONS

SPECIES NAME	CONCENTRATIONS: PRINTED ? (One value per layer) (0=No, 1=Yes)	CONCENTRATIONS: SAVED ON DISK ? (One value per layer) (0=No, 1=Yes)	DRY FLUXES: PRINTED ? (0=No, 1=Yes)	DRY FLUXES: SAVED ON DISK ? (0=No, 1=Yes)
! CO2	= 10 * 0	10 * 0	0	0 !
! HO2H	= 1,9 * 0	10 * 0	0	0 !
! RO2-HO2-PROD	= 10 * 0	10 * 0	0	0 !
! RO2-RO2-PROD	= 10 * 0	10 * 0	0	0 !
! -OOH	= 10 * 0	10 * 0	0	0 !
! -C	= 10 * 0	10 * 0	0	0 !
! -N	= 10 * 0	10 * 0	0	0 !
! H2	= 10 * 0	10 * 0	0	0 !
! H2SO4	= 10 * 0	10 * 1	0	0 !
! O3	=1,1,1,7 * 0	10 * 1	1	1 !
! NO	= 1,9 * 0	10 * 1	0	0 !
! NO2	= 1,9 * 0	10 * 1	0	0 !
! NO3	= 10 * 0	0, 9 * 0	0	0 !
! N2O5	= 10 * 0	0, 9 * 0	0	0 !
! HNO3	= 0, 9 * 0	0, 9 * 0	0	0 !
! HONO	= 10 * 0	0, 9 * 0	0	0 !
! HNO4	= 10 * 0	0, 9 * 0	0	0 !
! HO2	= 10 * 0	0, 9 * 0	0	0 !
! CO	= 10 * 0	0, 9 * 0	0	0 !
! RO2.	= 10 * 0	0, 9 * 0	0	0 !
! RCO3	= 10 * 0	0, 9 * 0	0	0 !
! PAN	= 1,7 * 0	0, 9 * 0	0	0 !
! HCHO	= 1,9 * 0	0, 9 * 0	0	0 !
! RNO3	= 10 * 0	0, 9 * 0	0	0 !
! MEK	= 10 * 0	0, 9 * 0	0	0 !
! CCHO	= 10 * 0	0, 9 * 0	0	0 !

```
! MGLY         =    10 * 0          ,      0, 9 * 0        ,            0           ,
! CRES         =    10 * 0          ,      0, 9 * 0        ,            0           ,
! AFG2         =    10 * 0          ,      0, 9 * 0        ,            0           ,
! AAR1         =    10 * 0          ,      0, 9 * 0        ,            0           ,
! AAR2         =    10 * 0          ,      0, 9 * 0        ,            0           ,
! AAR3         =    10 * 0          ,      0, 9 * 0        ,            0           ,
! AAR4         =    10 * 0          ,      0, 9 * 0        ,            0           ,
! ETHE         =    10 * 0          ,      0, 9 * 0        ,            0           ,
! OLE1         =    10 * 0          ,      0, 9 * 0        ,            0           ,
! SO2          =   1,9 * 0          ,        10 * 1        ,            1           ,

!END!

--------------------------------------------------------------------------------

INPUT GROUP: 8 -- Vertical and Horizontal Diffusivity Parameters
--------------


    HORIZONTAL DIFFUSIVITY:

       Method flag (KHMODE)                  Default: 3     ! KHMODE= 3 !
          KHMODE = 0 - PBL diffusivities are
                       determined based on stability
                       class (see DKHSTB array)
          KHMODE = 1 - Same as above except diffusivities
                       are adjusted for wind speed
          KHMODE = 2 - Uses Smagorinsky method
          KHMODE = 3 - Adds the results of methods 1 and 2

       Horizontal Diffusivity (m**2/s) above
       the DIFFBREAK height (DKHUP)          Default: 0.0  ! DKHUP = 0.0 !
       (USED ONLY IF KHMODE = 0, 1, or 3)

       Horizontal Diffusivity (m**2/s) below
       the DIFFBREAK height (DKHSTB(6))      Defaults: 224.,  96., 32.,  0.,  0., 0.
       (USED ONLY IF KHMODE = 0, 1, or 3)    ! DKHSTB = 224.,  96., 32.,  0.,  0., 0. !
       (NOTE: if KHMODE = 1 or 3, these
       DKHSTB values are scaled by wind speed)


    VERTICAL DIFFUSIVITY:

       Minimum vertical diffusivity (m**2/s)
       (DKZMIN)                              Default: 1.0  ! DKZMIN = 1.0 !

       Vertical diffusivity (m**2/s) at the
       model top (DKZTOP)                    Default: 0.0  ! DKZTOP = 0.0 !

!END!
```

assumed to be data, so no user comment information is allowed to appear within the delimiters. The inclusion in the control file of any variable that is being assigned its default value is optional.

The control file is organized into eight Input Groups preceded by a three line run title (see Table 4.1.1). The Input Groups must appear in order, i.e., Input Group 1 followed by Input Group 2, etc. However, the variables within an Input Group may appear in any order. The variable names in each Input Group are independent, so that the same name can be repeated in different Input Groups (e.g., as shown in the sample control file, species names (`S02`, `03`, etc) are use in several Input Groups). Each Input Group must end with an Input Group terminator consisting of the word `END` between two delimiters (i.e., `!END!`). Even a blank Input Group (i.e., one in which no variables are included) must end with an Input Group terminator in order to signal the end of that Input Group and the beginning of another.

The control file module has a list of variable names and array dimensions for each Input Group. Checks are performed to ensure that the proper variable names are used in each Input Group, and that no array dimensions are exceeded. Error messages result if an unrecognized variable name is encountered or too many values are entered for a variable.

A standard control file is provided along with the CALGRID test case run. It is recommended that a copy of the standard control file be permanently stored as a backup. Working copies of the control file may be made and then edited and customized by the user for a particular application.

Table 4.1.1. Control File Input Groups

INPUT GROUP	DESCRIPTION
*	Run Title First three lines of control file (up to 80 characters/line)
1	General Run Control parameters Starting date and hour, run length, time step, species counts, input file types, area source emissions distribution factors
2	Grid Control Parameters Grid types, number of cells, vertical layers, reference coordinates
3	Species List Species names, flags for determining which species are modeled, advected, emitted, and dry deposited
4	Dry Deposition Parameters - Gases Pollutant diffusivity, dissociation constant, reactivity, mesophyll resistance, Henry's law coefficient
5	Dry Deposition Parameters - Particles Geometric mass mean diameter, geometric standard deviation
6	Miscellaneous Dry Deposition Parameters Reference cuticle and ground resistances, reference pollutant reactivity, vegetation state
7	Output Options Printer control variables, disk output control variables
8	Horizontal and Vertical Diffusivity Parameters Horizontal diffusivity parameters, method flag, vertical diffusivity parameters

Control File Inputs - Input Group 1
General Run Control Parameters

VARIABLE	TYPE[a]	DESCRIPTION	DEFAULT VALUE
IBYR	I	Starting year of the CALGRID run (two digits)	-
IBMO	I	Starting month	-
IBDY	I	Starting day	-
IBHR	I	starting hour (00-23)	-
IRLG	I	Length of the run (hours)	-
NSUBTS	I	Number of time steps per hour (basic time step (seconds) = 3600./NSUBTS)	3
NSPEC	I	Total number of species (advected + steady-state species)	47
NSA	I	Number of species advected	36
NSDD	I	Number of species dry deposited	15
NSE	I	Number of species emitted	13
METHINT	I	Method flag for integration of the chemical mechanism (1 = Hybrid method, 2 - QSSA method)	2
ITICON	I	Initial concentration (ICON.DAT) file type 1 = formatted file containing one initial concentration value per layer per species 2 = unformatted file containing a full 3-D set of initial concentrations for each species	1
ITBCON	I	Lateral boundary condition (BCON.DAT) file type 1 = formatted file containing boundary types and time-independent boundary conditions as a function of height for each advected species 2 = unformatted file containing a full set of time-dependent boundary conditions for each boundary cell and species 3 = BCON.DAT file is not used. Time-independent boundary conditions are taken from the initial concentration distribution. Each boundary cell is assigned a concentration value equal to the adjacent non-boundary cell.	1

[a] I = Integer
R = Real

Control File Inputs - Input Group 1
General Run Control Parameters

VARIABLE	TYPE[a]	DESCRIPTION	DEFAULT VALUE
ITTCON	I	Top boundary condition (TCON.DAT) file type 1 = formatted file containing time-independent top boundary conditions for each advected species 2 = unformatted file containing a full set of time-dependent and space-dependent top boundary conditions for each advected species 3 = TCON.DAT file is not used. The top layer of the initial concentration distribution is used to obtain time-independent top boundary conditions	1
ITEM1	I	Flag for the file with stationary point sources with cyclical or constant emissions (`PTEMCYC.DAT`) 1 = Unformatted, direct-access `PTEMCYC.DAT` file is used 2 = `PTEMCYC.DAT` file is not used 3 = TCON.DAT file is not used. The top layer of the initial concentration distribution is used to obtain time-independent top boundary conditions	1

[a] I = Integer
R = Real

Control File Inputs - Input Group 1
General Run Control Parameters

VARIABLE	TYPE[a]	DESCRIPTION	DEFAULT VALUE
IEM1REC	I	Length of direct access records (bytes) used in the OPEN statement for the PTEMCYC.DAT file. The default value of 68 bytes is the length of data in the first record. If the record length is unknown, the model will open the file with an assumed record length of 68 bytes, read the first header record of the file, compute the actual record length, close and then re-open the file with the actual record length. However, this procedure does not work on all computer systems. It may be necessary for the user to compute and input the actual record length. If the host computer system requires the record length to be specified in the OPEN statement in words instead of bytes, a minor code modification may be necessary.	68
ITEM2	I	Flag for the file with stationary point sources with arbitrary emissions (PTEMARB.DAT) 1 = Unformatted PTEMARB.DAT file is used 2 = PTEMARB.DAT file is not used	1
ITEM3	I	Flag for the file with mobile point sources with constant emissions (PTEMMOB.DAT) 1 = Unformatted PTEMMOB.DAT file is used 2 = PTEMMOB.DAT file is not used	1
ITEM4	I	Flag for the file with area source emissions (AREM.DAT) 1 = Unformatted AREM.DAT file is used 2 = AREM.DAT file is not used	1
NZEM	I	Number of user-defined "emissions" layers (see Section 4.1.9)	2
ZFEM	R array	Height (m) of each emission layer face array (NZEM + 1 values must be entered)	0., 50., 100.

[a] I = Integer
R = Real

Control File Inputs - Input Group 1
General Run Control Parameters

VARIABLE	TYPE[a]	DESCRIPTION	DEFAULT VALUE
WTEM	R array	Fraction of area source emissions distributed in each user-defined "emissions" layer (NZEM values must be entered – one for each emissions layer) (Sum of all values of WTEM must be 1.0)	0.75, 0.25

[a] I = Integer
R = Real

Control File Inputs - Input Group 2
Grid Control Parameters

VARIABLE	TYPE[a]	DESCRIPTION	DEFAULT VALUE
NX	I	Number of grid cells in the X direction	-
NY	I	Number of grid cells in the Y direction	-
DGRID	R	Grid spacing (km)	-
XORIGKM	R	Reference UTM X coordinate (km) of the southwest corner of grid cell (1,1)	-
YORIGKM	R	Reference UTM Y coordinate (km) of the southwest corner of grid cell (1,1)	-
IUTMZN	I	UTM zone of coordinates	-
XLAT	R	Reference latitude (deg.) of the center of the modeling domain (used in solar elevation angle calculations)	-
XLONG	R	Reference longitude (deg.) of the center of the modeling domain	-
XTZ	R	Reference time zone of the center of the modeling domain (PST=8, MST=7, CST=6, EST=5)	-
IVGTYP	I	Vertical grid type 0 = uniform thickness above and below DIFFBREAK heights 1 = dynamically varying layer heights 2 = arbitrary fixed layer heights	2

[a] I = Integer
R = Real

Control File Inputs - Input Group 2
Grid Control Parameters

VARIABLE	TYPE[a]	DESCRIPTION	DEFAULT VALUE
NZ	I	Number of vertical layers (Used if IVGTYP = 0, 1, or 2)	-
NZL	I	Number of layers below DIFFBREAK (Used if IVGTYP = 0 or 1)	-
ZMINB	R	Minimum depth (m) of cells below DIFFBREAK and above layer #1 (Used if IVGTYP = 0)	20.
ZMAXB	R	Maximum depth (m) of cells below DIFFBREAK and above layer #1 (Used if IVGTYP = 0)	5000.
ZMINA	R	Minimum depth (m) of cells above DIFFBREAK (Used if IVGTYP = 0)	20.
ZMAXA	R	Maximum depth (m) of cells above DIFFBREAK (Used if IVGTYP = 0)	5000.
ZTOP	R	Top of modeling domain (m) (Used if IVGTYP = 0 or 1)	-
DZMIN	R	Minimum cell depth (m) for layers above layer #1 (Used if IVGTYP = 1)	20.
ZFACE	R array	Cell face heights (m) for the arbitrary grid (NZ + 1 values must be entered) (Used if IVGTYP = 2)	-
NZM	I	Number of vertical layers in the CALMET meteorological grid (i.e., no. layers of winds)	-

[a] I = Integer
R = Real

Control File Inputs - Input Group 3
Species List

Input Group 3 consists of a table containing four integer flags for each species. These flags indicate if a pollutant is modeled (0=no, 1=yes), advected (0=no, 1=yes), emitted (0=no, 1=yes), and dry deposited (0=no, 1=yes, treated as a gas with the resistance model, 2=yes, treated as a particle with the resistance model, or 3=yes, user-specified deposition velocities used).

The particular chemical mechanism used in the model determines which species are modeled (i.e., included in the chemistry), and advected. Steady-state species are "modeled" or computed internally within the chemistry module but are not subject to horizontal or vertical advection, diffusion, or dry deposition. The values provided in the standard control file for the modeled and advected flags should not be modified unless the chemical mechanism is also changed.

The user has control over which species are to be emitted and dry deposited in a particular run. If the dry deposition flag is set equal to 3 for any pollutant, a file called VD.DAT must be made available to the model. This file contains a diurnal cycle of 24 user-specified deposition velocities for each pollutant flagged (see Section 4.1.10).

The format of the species list table is:

```
                                                                  DRY
SPECIES          MODELED          ADVECTED          EMITTED       DEPOSITED
 NAME       (0=NO, 1=YES)    (0=NO, 1=YES)   (0=NO, 1=YES)  (0=NO,
                                                                  1=COMPUTED-GAS
                                                                  2=COMPUTED-PARTICLE
                                                                  3=USER-SPECIFIED)
! O3            =   1         ,       1         ,      0       ,      1      !
! NO            =   1         ,       1         ,      1       ,      0      !
! NO2           =   1         ,       1         ,      1       ,      0      !
```

The sample control file in Figure 4.1.1 contains a complete list of all the species included in the current chemical mechanism.

Control File Inputs - Input Group 4
Dry Deposition Parameters - Gases

Input Group 4 consists of a table containing the following five parameters which are required by the resistance deposition model for computing deposition velocities for gases:

- Pollutant diffusivity (cm^2/s) (see Eqn. 2.4-7)
- Aqueous phase dissociation constant, α_* (see Eqn. 2.4-14)
- Pollutant reactivity (see Eqn. 2.4-12)
- Mesophyll resistance, r_m (s/cm) (see Section 2.4)
- Henry's Law coefficient, H (dimensionless) (see Eqn. 2.4-14)

These parameters must be specified for each pollutant with a dry deposition flag of "1" in the species list (Input Group 3) indicating the use of the resistance model for a gas.

The format of the input table is shown below:

```
SPECIES     DIFFUSIVITY      ALPHA STAR      REACTIVITY    MESOPHYLL RESISTANCE     HENRY'S LAW COEFFI
 NAME        (cm**2/s)                                           (s/cm)              (dimensionless
-------     -----------      ----------      ----------    --------------------     ------------------
! HO2H =      0.2402     ,      1.00     ,      12.0    ,          0.0           ,          4.0e-7
! -OOH =      0.1403     ,      1.00     ,      12.0    ,          0.0           ,          1.0e-6
! O3   =      0.1594     ,     10.00     ,      15.0    ,          4.0           ,          2.0
! NO2  =      0.1656     ,      1.00     ,       8.0    ,          5.0           ,          3.5
! NO3  =      0.1656     ,      1.00     ,       8.0    ,          5.0           ,          1.0e-6
* HNO3 =      0.1628     ,      1.00     ,      18.0    ,          0.0           ,          8.0e-8
! HONO =      0.1100     ,      1.00     ,       4.0    ,          2.0           ,          4.3e-4
! HNO4 =      0.1500     ,      1.00     ,       4.0    ,          2.0           ,          1.0e-5
! HO2  =      0.2402     ,      1.00     ,      12.0    ,          0.0           ,          1.0e-6
! RO2. =      0.2402     ,      1.00     ,      12.0    ,          0.0           ,          1.0e-6
! PAN  =      0.1050     ,      1.00     ,       4.0    ,          1.0           ,          1.0e-2
! HCHO =      0.2336     ,      1.00     ,       4.0    ,          0.0           ,          4.0e-6
! RNO3 =      0.1100     ,      1.00     ,       4.0    ,          2.0           ,          1.0e-6
! SO2  =      0.1509     ,      1.00E3   ,       8.0    ,          0.0           ,          4.0e-2
```

Control File Inputs - Input Group 5
Dry Deposition Parameters - Particles

Input Group 5 consists of a table containing the geometric mass mean diameter (microns) and the geometric standard deviation (microns) required by the resistance deposition model for computing deposition velocities for particulate matter.

These parameters must be specified for each pollutant with a dry deposition flag of "2" in the species list (Input Group 3) indicating the use of the resistance model for a pollutant deposited as particulate matter Sulfuric acid (H_2SO_2) is generated from oxidation reactions involving SO_2. For purposes of computing dry deposition rates, H_2SO_2 is assumed to be in the form of particlate sulfate. In the current chemical mechanism, it is the only pollutant treated as a particle in the deposition calculations. The pollutant NO_3 refers to nitrogen trioxide, not particulate nitrate, and is deposited as a gas.

The format of the input table is shown below:

```
       *
SPECIES       GEOMETRIC MASS MEAN         GEOMETRIC STANDARD
 NAME              DIAMETER                    DEVIATION
                   (microns)                   (microns)
-------       -------------------         ------------------
! H2SO4   =          0.48           ,            2.00     !


*
 H2SO4 deposited as sulfate
```

Control File Inputs - Input Group 6
Miscellaneous Dry Deposition Parameters

VARIABLE	TYPE[a]	DESCRIPTION	DEFAULT VALUE
RCUTR	R	Reference cuticle resistance (s/cm) (see Eqn. 2.4-13)	17.
RGR	R	Reference ground resistance (s/cm) (see Eqn. 2.4-13)	5.
REACTR	R	Reference pollutant reactivity (see Eqn. 2.4-12)	8.
IVEG	I	Vegetation state in unirrigated areas 1 = vegetation is active and unstressed 2 = vegetation is active and stressed 3 = vegetation is inactive	-

[a] I = Integer
R = Real

Control File Inputs - Input Group 7
Output Options

VARIABLE	TYPE[a]	DESCRIPTION	DEFAULT VALUE
ICON	I	Control variable for creation of an output disk file (`ICON.DAT`) containing hourly concentrations fields (species stored in this file are controlled by the output species table described below). 0 = do not create `ICON.DAT`, 1 = create `ICON.DAT`	1
IDRY	I	Control variable for creation of an output disk file (`DFLX.DAT`) containing hourly dry flux fields (species stored in this file are controlled by the output species table described below). 0 = do not create `DFLX.DAT`, 1 = create `DFLX.DAT`	1
ICPRT	I	Control variable for printing of concentration fields to the output list file (`CALGRID.LST`).	0

[a] I = Integer
R = Real

Control File Inputs - Input Group 7
Output Options

VARIABLE	TYPE[a]	DESCRIPTION	DEFAULT VALUE
		0 = do not print any concentrations, 1 = print concentrations indicated in output species table	
IFPRT	I	Control variable for printing of dry flux fields to the output list file (`CALGRID.LST`). 0 = do not print any dry fluxes, 1 = print dry fluxes indicated in output species table	0
ITPRT	I	Control variable for printing of fluxes out of the top of the model 0 = do not print any top fluxes, 1 = print all top fluxes	0
IVDPRT	I	Control variable for printing of gridded fields of dry deposition velocities 0 = do not print any dry deposition velocities 1 = print dry deposition velocities for all deposited pollutants	0
IEPRT	I	Control variable for printing of gridded fields of total (area + point source) emission rates. IEPRT is the number of layers, starting at the lowest layer, to print. If IEPRT is 0, no emissions are printed. If IEPRT is set equal to NZ, emissions for all NZ layers will be printed (NOTE: IEPRT must be less than or equal to NZ).	0
ICFRQ	I	Printing interval for the concentration fields. Concentrations are printed every "ICFRQ" hours. (Used only if ICPRT = 1).	1
IFFRQ	I	Printing interval for the dry flux fields. Dry fluxes are printed every "IFFRQ" hours. (Used only if IFPRT = 1).	1
ITFRQ	I	Printing interval for the top flux fields. Top fluxes are printed every "ITFRQ" hours. (Used only if ITPRT = 1).	1

[a] I = Integer
R = Real

Control File Inputs - Input Group 7
Output Options

VARIABLE	TYPE[a]	DESCRIPTION	DEFAULT VALUE
IVDFRQ	I	Printing interval for the gridded deposition velocity fields. Deposition velocities are printed every "IVDFRQ" hours. (Used only if IVDPRT = 1).	1
IEFRQ	I	Printing interval for the gridded emissions fields. The emissions are printed every "IEFRQ" hours. (Used only if IEPRT = 1).	1

[a] I = Integer
R = Real

Control File Inputs - Input Group 7
Output Options

In addition to the variables described above, Input Group 7 also contains a table of species with a series of flags indicating for each pollutant, which layers of the concentrations fields are to be printed, and stored in the concentration disk output file (`ICON.DAT`), and which dry fluxes are to be printed and stored in the dry flux disk output file (`DFLX.DAT`). A total of 2*NZ+2 integer flags are required for each pollutant. The first NZ values determine which layers of the concentration field for a given pollutant are printed (O=not printed, 1=printed). The next NZ values determine which layers of the concentration are stored in the output file. The final two variables determine if the dry flux field for the pollutant is printed and saved on disk, respectively. (A value of 0 indicates “no”, and a value of 1 indicates “yes”).

The format of the species output table is:

SPECIES LIST FOR OUTPUT OPTIONS

SPECIES NAME	CONCENTRATIONS: PRINTED ? (One value per layer) (0=No, 1=Yes)	CONCENTRATIONS: SAVED ON DISK ? (One value per layer) (0=No, 1=Yes)	DRY FLUXES: PRINTED ? (0=No, 1=Yes)	DRY FLUXES: SAVED ON DISK ? (0=No, 1=Yes)
! O3	=1,1,1,7 * 0 ,	10 * 1 ,	1 ,	1 !
! NO	= 1,9 * 0 ,	10 * 1 ,	0 ,	0 !
! NO2	= 1,9 * 0 ,	10 * 1 ,	0 ,	0 !
! NO3	= 10 * 0 ,	0, 9 * 0 ,	0 ,	0 !
! N2O5	= 10 * 0 ,	0, 9 * 0 ,	0 ,	0 !
! HNO3	= 0, 9 * 0 ,	0, 9 * 0 ,	0 ,	0 !
! HONO	= 10 * 0 ,	0, 9 * 0 ,	0 ,	0 !

Control File Inputs - Input Group 8
Horizontal and Vertical Diffusivity Parameters

VARIABLE	TYPE[a]	DESCRIPTION	DEFAULT VALUE
KHMODE	I	Method for computing horizontal diffusivities 0 = Diffusivities within the boundary layer are determined based on the PGT stability class for each grid cell. Diffusivities above the boundary layer are determined by the variable DKHUP described below. 1 = Same as above except diffusivities are scaled by the wind speed 0 = The Smagorinsky method is used to determine horizontal diffusivities 0 = Results of methods 1 and 2 are added	3
DKHUP	R	Horizontal diffusivity applied above the boundary layer (above DIFFBREAK height) (Used only if KHMODE = 0, 1, or 3)	0.0
DKHSTB	R array	Horizontal diffusivity (m^2/s) within the boundary layer for each PGT stability class (6 values must be entered) (Used only if KHMODE= 0, 1. or 3) * Default values: 224., 96., 32., 0., 0., 0.	*
DKZMIN	R	Minimum vertical diffusivity (m^2/s)	1.0
DKZTOP	R	Vertical diffusivity (m^2/s) at the model top	0.0

[a] I = Integer
R = Real

4.1.2 Meteorological Data File (CALMET.DAT)

The CALMET.DAT file contains the meteorological data fields required to drive the CALGRID model. It also contains certain geophysical fields, such as terrain elevations, surface roughness, lengths, and land use types, used by both the CALMET meteorological model and CALGRID. Although the input requirements of CALGRID are designed to be directly compatible with CALMET meteorological fields produced by other meteorological models can be substituted for the CALMET output as long as the required variables are produced and the output is reformatted to be consistent with the CALMET.DAT file specifications described in this section.

CALMET.DAT File - Header Records

The CALMET.DAT file consists of a set of up to fourteen header records, followed by a set of hourly data records. The header records contains a descriptive title of the meteorological run, Information including the horizontal and vertical grid systems of the meteorological grid, the number, type, and coordinates of the meteorological stations included in the CALMET run, gridded fields of surface roughness lengths, land use, terrain elevations, leaf area indexes, and a pre-compute field of the closest surface meteorological station number to each grid point.

The actual number of header records may vary because, as explained below, records containing surface, upper air, and precititation station coordinates are not included if these stations were not included in the run.

The horizontal grid system used in the meteorological modeling must match that used in the CALGRID simulation. However, the fixed vertical layers used in the meteorological modeling do not need to (and in most applications will not) match those used in the CALGRID run, which allows variable as well as fixed vertical grid systems.

The following variables stored in the CALMET.DAT header records are checked in the setup phase of the CALGRID model run to ensure compatibility with variables specified in the CALGRID control file: number of grid cells in the X and Y directions, grid size, reference UTM coordinates of the grid origin, and UTM zone of the grid origin.

In addition, a check is made that the number of surface stations does not exceed the array dimension parameter, MXSS, contained in the CALGRID parameter file, PARAMS.GRD. (Several meteorological parameters observed or computed at surface meteorological stations are stored in the CALMET.DAT file and require properly sized arrays to store them). Currently, MXSS is set to allow up to 50 surface stations. If necessary, MXSS can be increased by editing the PARAMS.GRD

file and recompiling the CALGRID program. It should be noted that the value of MXSS in PARAMS.GRD need not match the parameter of the same name in the CALMET parameter file. It need only be greater than or equal to the actual number of surface stations used in the CALMET run.

Sample Fortran read statements for the CALMET.DAT header records are:

```
c --- Header record 1 -- Run title
      READ(iunit)TITLE


c --- Header record 2 -- General run and grid information

      READ(iunit)VERMET, LEVMET, IBYR, IBMO, IBDY, IBHR, IBTZ, IRLG,
     1 IRTYPE, NXK, NYM, NZM, XGRIDM, XORIGM, YORIGM, IUTMZNM, IWFCOD,
     2 NSSTA, MUSTA, NPSTA, NOWSTA, NLU, IWATi, IWAT2, LCALGRD


c --- Header record 3 -- Vertical cell face heights (nz+1 values)
      READ(iunit)CLAB1,ZFACEM


c --- Header records 4 and 5 -- Surface station coordinates
      if(nssta. gt. O)then
        READ(iunit)CLAB2,XSSTA
        READ(iunit)CLAB3,YSSTA
      end if
c --- Header records 6 and 7 -- Upper air station coordinates
      if(nusta.gt.0)then
        READ(iunit)CLAB4, XUSTA
        READ(junit)CLAB5, YUSTA
      endif

c --- Header records 8 and 9-- Precipitation station coordinates
      if(npsta.gt.0)then
        READ(iunit)CLAB6, XPSTA
        READ(iunit)CLAB7, YPSTA
      end if

c --- Header record 10 -- Surface roughness lengths

      READ(iunit)CLAB8,ZO

c --- Header record 11 -- Land use categories
```

```
      READ(iunit)CLAB9,ILANDU

c --- Header record 12 -- Terrain elevations
      READ(iunit)CLABl0,ELEV

c --- Header record 13 - Leaf area indexes
      READ(iunit)CLAB11,XLAI

C --- Header record 14 - Nearest surface station to each grid point
      READ(iunit)CLAB12,NEARS
```

where the following declarations apply:

```
      real ZFACEM(nzm+1),XSSTA(nssta),YSSTA(nssta)
      real XUSTA(nusta),YUSTA(nusta)
      real XPSTA(npsta),YPSTA(npsta)
      real ZO(nxm,nym),ELEV(nxm,nym),XLAI(nxm,nym)
      integer ILANDU(nxm,nym),NEARS(nxm,nym)
      character*8O TITLE(3)
      character*8 VERMET,LEVMET,CLAB1,CLAB2,CLAB3,CLAB4,CLAB5
      character*8 CLAB6,CLAB7,CLAB8,CLAB9,CLABlO,CLAB1l,CLAB12
      logical LCALGRD
```

CALMET.DAT File - Header Records

HEADER REC. NO.	VAR. NO.	VAR. NAME	TYPE[a]	DESCRIPTION
1	1	TITLE	C*80 array	Array with three 80-character lines of the user's title of the CALMET run
2	1	VERMET	C*8	CALMET model version number
2	2	LEVMET	C*8	CALMET model level number
2	3	IBYR	I	Starting year of CALMET run
2	4	IBMO	I	Starting month
2	5	IBDY	I	Starting day
2	6	IBHR	I	Starting hour
2	7	IBTZ	I	Base time zone (05=EST, 06=C-ST, 07=MST, 08=PST)
2	8	IRLG	I	Run length (hours)

[a]C*80 = Character*80
C*8 = Character*8
I = Integer
R = Real

CALMET.DAT File - Header Records

HEADER REC. NO.	VAR. NO.	VAR. NAME	TYPE[a]	DESCRIPTION
2	9	IRTYPE	I	Run type (must be run type 1 to drive CALGRID)
2	10	NXM	I	Number of grid cells in the X direction
2	11	NYM	I	Number of grid cells in the Y direction
2	12	NZM	I	Number of vertical layers
2	13	XGRIDM	R	Grid spacing (m)
2	14	XORIGM	R	UTM X coordinate (m) of southwest corner of grid point (1,1)
2	15	YORIGM	R	UTM Y coordinate (m) of southwest corner of grid point (1,1)
2	16	IUTMZNM	I	UTM zone of coordinates

[a]C*80 = Character*80
C*8 = Character*8
I = Integer
R = Real

CALMET.DAT File - Header Records

HEADER REC. NO.	VAR. NO.	VAR. NAME	TYPE[a]	DESCRIPTION
2	17	IWFCOD	I	Wind field module used (0=objective analysis, 1=diagnostic model)
2	18	NSSTA	I	Number of surface meteorological stations
2	19	NUSTA	I	Number of upper air stations
2	20	NPSTA	I	Number of precipitation stations

[a]C*8 = Character*8
I = Integer
R = Real
L = Logical
[b]Included only if NSSTA $>$ 0

CALMET.DAT File - Header Records

HEADER REC. NO.	VAR. NO.	VAR. NAME	TYPE[a]	DESCRIPTION
2	21	NOWSTA	I	Number of overwater stations
2	22	NLU	I	Number of land use categories
2	23	IWAT1	I	Range of land use categories
2	24	IWAT2	I	corresponding to water surfaces (IWAT1 to IWAT2, inclusive)
2	25	LCALGRD	L	Flag Indicating if special meteorological parameters required by CALGRID are contained in the file (LCALGRD must be TRUE to drive CALGRID)
3	1	CLAB1	C*8	Variable label ('ZFACE')
3	2	ZFACEM	R array	Heights (m) of cell faces (NZM + 1 values)
4[b]	1	CLAB2	C*8	Variable label ('XSSTA')
4[b]	2	XSSTA	R array	X UTM coordinates (m) of each surface met. station

[a] C*8 = Character*8
I = Integer
R = Real
L = Logical

[b] Included only if NSSTA > 0

CALMET.DAT File - Header Records

HEADER REC. NO.	VAR. NO.	VAR. NAME	TYPE[a]	DESCRIPTION
5[b]	1	CLAB3	C*8	Variable label ('YSSTA')
5[b]	2	YSSTA	R array	Y UTM coordinates (m) of each surface met. station
6[c]	1	CLAB4	C*8	Variable label ('XUSTA')
6[c]	2	XUSTA	R array	X UTM coordinates (m) of each upper air met. station
7[c]	1	CLAB5	C*8	Variable label ('YUSTA')
7[c]	2	YUSTA	R array	Y UTM coordinates (m) of each upper air met. station
8[d]	1	CLAB6	C*8	Variable label ('XPSTA')
8[d]	2	XPSTA	R array	X UTM coordinates (m) of each precipitation station
9[d]	1	CLAB7	C*8	Variable label ('YPSTA')
9[d]	2	YPSTA	R array	Y UTM coordinates (m) of each precipitation station
10	1	CLAB8	C*8	Variable label ('ZO')
10	2	ZO	R array	Gridded field of surface roughness lengths (m)
11	1	CLAB9	C*8	Variable label ('ILANDU')
11	2	ILANDU	R array	Gridded field of land use category for each grid cell

[a]C*8 = Character*8
I = Integer
R = Real
L = Logical

[b]Included only if NSSTA > 0

[c]Included only if NUSTA > 0

[d]Included only if NPSTA > 0

CALMET.DAT File - Header Records

HEADER REC. NO.	VAR. NO.	VAR. NAME	TYPE[a]	DESCRIPTION
12	1	CLAB10	C*8	Variable label ('ELEV')
12	2	ELEV	R array	Gridded field of terrain elevations for each grid cell
13	1	CLAB11	C*8	Variable label ('XLAI')
13	2	XLAI	R array	Gridded field of leaf area index for each grid cell
14	1	CLAB12	C*8	Variable label ('NEARS')
14	2	NEARS	R array	Nearest surface met. station to each grid point

[a]C*8 = Character*8
I = Integer
R = Real

CALMET.DAT File - Data Records

The CALMET.DAT data records include hourly fields of winds and meteorological variables. In additional to the regular CALMET output variables, CALGRID requires three-dimensional fields of the vertical velocity and air temperature The presence of these fields in the CALMET output file is flagged by the header record logical variable, LCALGRD, having a value of TRUE.

The data records contain three-dimensional gridded fields of U, V, and W wind components and air temperature, two-dimensional fields of PGT stability class, surface friction velocity, mixing height, Monin-Obukhov length, convective velocity scale, and precipitation rate (not used by CALGRID), and values of the temperature, air density, short-wave solar radiation, relative humidity, and precipitation type codes (not used by CALGRID) defined at the surface meteorological stations.

Sample Fortran read statements for the CALMET.DAT data records are:

```
c --- Read U, V, W wind components

C     Loop over vertical layers, k

      READ(iunit)CLABU,((UMET(i,j,k),i=1,nxm),j=i,nym)
      READ(iunit)CLABV,((VMET(i,j,k),i=l,nxm)1j=l,nym)
      if(LCALGRD)READ(iunit)CLABW,((WMET(i,j,k),i=i,nxm),j=i,nym)

C     End loop over vertical layers

c --- Read 3-D temperature field
      if (LCALGRD)

C     Loop over vertical layers, k

        READ(iunit)CLABT,((TMET(1,j,k)1i=i,nxm),j=i,nym)

C     End loop over vertical layers
      endif

C --- Read 2-D meteorological fields

      READ(iunit)CLABSC,IPGT
      READ(lunit)CLABUS,USTAR
      READ(iunit)CLABZI,HTMIX
      READ(iunit)CLABL,XMONIN
      READ(iunit)CLABWS,WSTAR
      READ(iunit)CLABRMM,RMM
```

```
C Read l-D variables defined at surface met. stations
      READ(iunit)CLABTK,TEMPSS
      READ(iunit)CLABD,RHOSS
      READ(iunit)CLABQ,QSWSS
      READ(iunit)CLABRH,IRHSS
      READ(iunit)CLABPC,IPCODE
```

where the following declarations apply:

```
      real UMET(nxm,nym,nzm),VMET(nxm,nym,nzm),WMET(nxm,nym,nzm)
      real TMET(nxm, nym, nzm)
      real USTAR(nxm,nym),HTMIX(nxm,nym),XMONIN(nxm,nym)
      real WSTAR(nxm,nym),RMM(nxm,nym)
      real TEMPSS(nssta),RHOSS(nssta),QSWSS(nssta)
      integer IPGT(nxm,nym)
      integer IRHSS(nssta),IPCODE(nssta)
      character*8 CLABU, CLABV, CLABW, CLABT, CLABSC, CLABUS, CLABZI
      character*8 CLABL, CLABWS, CLABRMM, CLABTK, CLABD, CLABQ, CLABRH
      character*8 CLABPC
```

CALMET.DAT File - Data Records

HEADER REC. NO.	VAR. NO.	VAR. NAME	TYPE[a]	DESCRIPTION
1	1	CLABU	C*8	Variable label ('U-LEVxxx', where xxx indicates the layer number)
1	2	UMET	R array	U-component (m/s) of the winds at each grid point
2	1	CLABV	C*8	Variable label ('V-LEVxxx', where xxx indicates the layer number)
2	2	VMET	R array	V-component (m/s) of the winds at each grid point
3[b]	1	CLABW	C*8	Variable label ('W-LEVxxx', where xxx indicates the layer number)

[a] C*8 = Character*8
I = Integer
R = Real

[b] Record types 3 and 4 are included only if LCALGRD is TRUE

CALMET.DAT File - Data Records

HEADER REC. NO.	VAR. NO.	VAR. NAME	TYPE[a]	DESCRIPTION
3[b]	2	WMET	R array	W-component (m/s) of the winds at each grid point
(Record types 1, 2, 3 repeated NZM times (once per layer) as a set)				
4[b]	1	CLABT	C*8	Variable label ('T-LEVxxx', where xxx indicates the layer number)
4[b]	2	TMET	R array	Air temperature (deg. K) at each grid point
(Record type 4 repeated NZM times (once per layer))				
5	1	CLABSC	C*8	Variable label ('IPGT')
5	2	IPGT	I array	PGT stability class
6	1	CLABUS	C*8	Variable label ('USTAR')
6	2	USTAR	R array	Surface friction veclocity (m/s)
7	1	CLABZI	C*8	Variable label ('ZI')
7	2	HTMIX	R array	Mixing height (m)

[a]C*8 = Character*8
I = Integer
R = Real
[b]Record types 3 and 4 are included only if LCALGRD is TRUE

CALMET.DAT File - Data Records

HEADER REC. NO.	VAR. NO.	VAR. NAME	TYPE[a]	DESCRIPTION
8	1	CLABL	C*8	Variable label ('EL')
8	2	XMONIN	R array	Monin-Obukhov length (m)
9	1	CLABWS	C*8	Variable label ('WS')
9	2	WSTAR	R array	Convective velocity scale (m/s)
10	1	CLABRMM	C*8	Variable label ('RMM')

[a]C*8 = Character*8
I = Integer
R = Real

CALMET.DAT File - Data Records

HEADER REC. NO.	VAR. NO.	VAR. NAME	TYPE[a]	DESCRIPTION
10	2	RMM	R array	Precipitation rate (mm/hr). Not used by CALGRID.
11	1	CLABTK	C*8	Variable label ('TEMPK')
11	2	TEMPSS	R array	Temperature (deg. K) at each surface met. station
12	1	CLABD	C*8	Variable label ('RHO')
12	2	RHOSS	R array	Air density (kg/m^3) at each surface met. station
13	1	CLABQ	C*8	Variable label ('QSW')
13	2	QSWSS	R array	Short-wave solar radiation (W/m^2) at each surface met. station
14	1	CLABRH	C*8	Variable label ('IRH')
14	2	IRHSS	R array	Relative humidity (percent) at each surface met. station
15	1	CLABPC	C*8	Variable label ('IPGT')
15	2	IPCODE	R array	Percipitation type code (not used by CALGRID)

[a] C*8 = Character*8
I = Integer
R = Real

4.1.3 Initial Concentration Data File (ICON.DAT)

The ICON.DAT data file contains the initial concentrations required to begin the CALGRID simulation. Two options, controlled by the control file variable ITICON, are provided for the input of the initial concentration field.

ITICON = 1	for a formatted input file containing one concentration value per layer per species.
ITICON = 2	for an unformatted file containing a full 3-D set of initial concentrations for each species.

Formatted Initial Concentration File

The formatted initial concentration file is intended to provide a simple way to initialize the concentration fields in the model. The user inputs a single value of the concentration for each vertical layer and advected species in the simulation. CALGRID internally assigns this value to each of the NX*NY grid cells in a given layer. The initial concentrations are specified in units of ppm.

An example of a formatted ICON.DAT data file is shown in Table 4.1.3. The formatted ICON file uses a.control file format (see Section 4.1.1). All text outside the delimiters (!) is considered as user comment information and is echoed back but otherwise ignored by the input module. Each data line consists of a delimiter followed by the species name (e.g., O3, SO2, etc.), "NZ" initial concentration values corresponding to layers 1 through NZ (layer 1 being the lowest layer, layer "NZ" the top layer), and a terminating delimiter. The data may extend over more than one line. The line being continued must end with a comma. The use of repetition factors is allowed (e.g., 3*1.0 instead of 1.0, 1.0, 1.0). The file must end with an input group terminator (i.e., !END!).

Formatted Initial Concentration File (ICON.DAT)

Initial values of the concentration are specified for each advected species (i.e., "Build-up" and "active" species only– steady-state species are not advected). One concentration value is read per layer for each advected species.

This file is used only if ITICON = 1 in the control file. If ITICON = 2, an unformatted file containing a full 3-D set of concentrations (NX*NY*NZ values) for each species is read.

```
SPECIES            Initial Concentration (ppm) for each layer
 NAME                     (NZ values must be entered)
-------            -------------------------------------------
```

```
BUILD-UP SPECIES

! CO2          =       10 * 0.51E-13,          !
! HO2H         =       10 * 0.23E-13,          !
! RO2-HO2-PROD =       10 * 0.23E-13,          !
! RO2-HO2-PROD =       10 * 0.23E-13,          !
! -OOH         =       10 * 0.23E-13,          !
! -C           =       10 * 0.23E-13,          !
! -N           =       10 * 0.23E-13,          !
! H2           =       10 * 0.11E-11,          !
! H2SO4        =       10 * 0.23E-13,          !

ACTIVE SPECIES

! O3           =       10 * 0.47E-13           !
! NO           =       10 * 0.60E-01           !
! NO2          =       10 * 0.20E-01           !
! NO3          =       10 * 0.36E-13           !
! N2O5         =       10 * 0.21E-13           !
! HNO3         =       10 * 0.36E-13           !
! HONO         =       10 * 0.48E-13           !
! HNO4         =       10 * 0.29E-13           !
! HO2          =       10 * 0.68E-13           !
! CO           =       10 * 2.12               !
! RO2.         =       10 * 0.23E-13           !
! RCO3.        =       10 * 0.30E-13           !
! PAN          =       10 * 0.19E-13           !
! HCHO         =       10 * 0.65E-02           !
! RNO3         =       10 * 0.17E-13           !
! MEK          =       10 * 0.35E-02           !
! CCHO         =       10 * 0.33E-02           !
! MGLY         =       10 * 0.31E-13           !
! CRES         =       10 * 0.63E-01           !
! AFG2         =       10 * 0.31E-13           !
! AAR1         =       10 * 0.012              !
! AAR2         =       10 * 0.22E-01           !
! AAR3         =       10 * 0.11E-01           !
! AAR4         =       10 * 0.63E-01           !
! ETHE         =       10 * 0.30E-01           !
! OLE1         =       10 * 0.33E-01           !
! SO2          =       10 * 0.96E-01           !

!END!
```

The model checks that values have been entered for every species and layer in the model run An error message is printed and execution of the run is terminated if any values are missing. The run will terminate with an error message from the input routine if too many values are entered (e.g., more than "NZ" values for a particular species). Also, the species names must match those used in the chemical mechanism of the model.

Unformatted Initial Concentration File

The unformatted initial concentration file allows the user to specify a full three-dimensional field of initial concentrations for each species. This may be the output of a previous modeling run (suitably reformatted) or the result of an analysis of observational data. The control file variable, `ITICON`, must be set equal to 2 in order to use the unformatted file option.

The unformatted `ICON.DAT` file consists of one data record for each advected species. Each data record contains a 12-character species name followed by NX*NY*NZ concentration values, where NX and NY are the number of grid cells in the X and Y directions, and NZ is the number of layers. The species names must match those used in the chemical mechanism of the model and be in the same order within the file. The file contains a total of NSA records, where NSA is the number of advected species. The initial concentrat1ons are specified in units of ppm.

Sample Fortran read statements for the unformatted initial concentration file are:

```
Loop over species

READ(iunit)CLAB,XINIT

End loop over species
```

where the following declarations apply:

```
character*l2 CLAB
real XINIT(nx,ny,nz)
```

Unformatted `ICON.DAT` File - Data Records

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	CLAB	C*12	Species identified (up to 12 characters)
NEXT	XINIT	R	Initial concentrations (ppm) for each grid
NX*NY*NZ		Array	cell

[a]C*12 = Character*12
R = Real

4.1.4 Lateral Boundary Condition Data File (BCON.DAT)

The BCON.DAT data file contains lateral boundary concentrations for each advected species. Three options, controlled by the control file variable ITBCON, are provided for the input of the lateral boundary conditions.

ITBCON = 1	for a formatted input file containing boundary types and time-independent boundary conditions as a function of height for each advected species.
ITBCON = 2	for an unformatted file containing a complete set of time-dependent boundary conditions for each advected species. Each boundary cell can have a different value for each time step with this option.
ITBCON = 3	if the BCON.DAT file is not used. The boundary conditions are taken from the initial concentration file. The value at each boundary cell is set equal to the initial concentration at the adjacent inner cell. These boundary condition values are time-independent.

Formatted Lateral Boundary Condition File

The formatted boundary condition file (i.e., ITBCON=1) contains two parts. In the first part, the user specifies the number of boundary types and assigns a boundary type to each boundary cell. For example, the user may categorize the boundaries as having three types of inflow concentrations. Boundary cells over water with "clean" inflow concentrations can be classified as "boundary type 1". Boundary cells over land can be classified as having "moderate" (boundary type 2) or "high" (boundary type 3) inflow concentrations.

The maximum number of boundary types allowed is determined by the parameter MXBTYP in the parameter file, PARAMS.GRD. Currently, MXBTYP is set to allow up to 10 boundary types. However, MXBTYP can be easily modified by the user by editing the PARAMS.GRD file and recompiling the CALGRID program.

The second part of the formatted BCON.DAT input file contains one time-independent concentration for each boundary type, vertical layer, and species. The concentrations are specified in units of ppm.

An example of a formatted BCON.DAT data file is shown in Table 4.1.4. The formatted BCON.DAT file uses a control file format (see Section 4.l.l). All text outside the delimiters (!) is considered as user comment information and is echoed back but otherwise ignored by the input module. In the first part of the file, each

line of boundary type data consists of a delimiter followed by the character "B-TYPE=", the integer boundary types for the boundary cells in that row, a terminating delimiter, and an input group terminator (!END!). The Y index values outside the delimiters shown in the example are optional. It is necessary to end each row of boundary types with an input group terminator because each row is internally treated as one input group. Note that NBTYPE (number of boundary types) is part of the input group containing the first row of data and therefore does not end with an input group terminator.

The species data in the second part of the file consists of a delimiter followed by the species name (e.g., O3, SO2, etc.) and NZ values for each boundary type. The data may extend over more than one line. The line being continued must end with a comma. The control file format allows the use of repetition factors (e.g., 3 * 1.0 instead of 1.0, 1.0, 1.0). The second part of the file needs only one input group terminator at the end of the file.

The boundary types must be entered with decreasing values of Y down (i.e., north at the top, south at the bottom) and increasing values of X to the right (i,e., west to the left, east to the right). The ordering of species in Part 2 of the file is unimportant. However, NBTYPE*NZ values must be entered for each species (NZ is the number of vertical layers).

The model checks that values have been entered for every advected species and boundary type. Missing values will result in an error message and termination of the run. The species names must match those used by the chemical mechanism of the model.

Unformatted Lateral Boundary Condition File

The unformatted lateral boundary condition file allows the user to specify different time-dependent boundary condition values for each boundary cell. The control file variable, ITBCON, is set equal to 2 in order to flag the use of the unformatted file option.

The unformatted BCON.DAT file consists of two header records followed by a set of data records. Each data record set contains a record specifying the time period for which the data is valid, followed by NSA*NZ records with the boundary values for each species and layer (NSA is the number of advected speciess NZ is the number of vertical layers). The time intervals at which the boundary values are updated can be hourly or any multiple hour period, and can vary from record to record within the file.

Table 4.1.4 Sample formatted lateral boundary condition file (BCON.DAT) for a 19 x 22 grid with six vertical layers. Three boundary types (low, moderate, and high inflow concentrations) are used. (Page 1 of 2).

FORMATTED BOUNDARY CONDITION FILE (BCON)

Boundary values of the concentration are specified for each advected species, layer and boundary type (i.e., "Build-up" and "active" species).

This file is used only if ITBCON = 1 in the control file. If ITBCON = 2, an unformatted file containing hourly boundary conditions is read. If ITBCON = 3, boundary conditions are taken from the initial concentration field, and the BCON file is not used.

PART 1 -- Define the BOUNDARY TYPE for each boundary cell

Number of boundary types (NBTYPE) No default ! NBTYPE = 3 !

* Y Index		X Index																	
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18 19
22	! BTYPE =	1,	1,	1,	1,	1,	2,	2,	2,	2,	2,	2,	2,	2,	2,	2,	2,	2,	2 ! !END!
21	! BTYPE =	1,																	2 ! !END!
20	! BTYPE =	1,																	2 ! !END!
19	! BTYPE =	1,																	2 ! !END!
18	! BTYPE =	1,																	2 ! !END!
17	! BTYPE =	1,																	2 ! !END!
16	! BTYPE =	1,																	3 ! !END!
15	! BTYPE =	1,																	3 ! !END!
14	! BTYPE =	1,																	3 ! !END!
13	! BTYPE =	1,																	3 ! !END!
12	! BTYPE =	1,																	3 ! !END!
11	! BTYPE =	1,																	3 ! !END!
10	! BTYPE =	1,																	3 ! !END!
9	! BTYPE =	1,																	3 ! !END!
8	! BTYPE =	1,																	3 ! !END!
7	! BTYPE =	1,																	3 ! !END!
6	! BTYPE =	1,																	3 ! !END!
5	! BTYPE =	1,																	3 ! !END!
4	! BTYPE =	1,																	3 ! !END!
3	! BTYPE =	1,																	3 ! !END!
2	! BTYPE =	1,																	3 ! !END!
1	! BTYPE =	1,	1,	1,	1,	1,	1,	1,	1,	1,	3,	3,	3,	3,	3,	3,	3,	3,	3 ! !END!

---

* NOTE: Y must be entered decreasing downward.

Table 4.1.4 Sample formatted lateral boundary condition file (BCON.DAT) for a 19 x 22 grid with six vertical layers. Three boundary types (low, moderate, and high inflow concentrations) are used. (Page 2 of 2).

```
-----------------------------------------------------------------
PART 2 -- Specify the BOUNDARY CONDITION for each boundary type
          and layer
-----------------------------------------------------------------


SPECIES
 NAME              I----- Type 1 -----I----- Type 2 -----I----- Type 3 -----I
-------                  (NZ values)        (NZ values)        (NZ values)

BUILD-UP SPECIES
! CO2          =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! HO2H         =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! RO2-HO2-PROD =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! RO2-RO2-PROD =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! -OOH         =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! -C           =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! -N           =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! H2           =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! H2SO4        =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
ACTIVE SPECIES
! O3           =       6 * 0.005,          6 * 0.010,         6 * 0.015       !
! NO           =       6 * 0.001,          6 * 0.005,         6 * 0.010       !
! NO2          =       6 * 0.0001,         6 * 0.0005,        6 * 0.001       !
! NO3          =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! N2O5         =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! HNO3         =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! HONO         =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! HNO4         =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! HO2          =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! CO           =       6 * 0.5   ,         6 * 1.0   ,        6 * 2.0         !
! RO2.         =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! RCO3.        =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! PAN          =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! HCHO         =       6 * 0.003 ,         6 * 0.006 ,        6 * 0.010       !
! RNO3         =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! MEK          =       6 * 0.002 ,         6 * 0.004 ,        6 * 0.006       !
! CCHO         =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! MGLY         =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! CRES         =       6 * 0.005 ,         6 * 0.007 ,        6 * 0.009       !
! AFG2         =       6 * 1.e-15,         6 * 1.e-15,        6 * 1.e-15      !
! AAR1         =       6 * 0.050 ,         6 * 0.100 ,        6 * 0.200       !
! AAR2         =       6 * 0.010 ,         6 * 0.020 ,        6 * 0.050       !
! AAR3         =       6 * 0.005 ,         6 * 0.010 ,        6 * 0.020       !
! AAR4         =       6 * 0.005 ,         6 * 0.010 ,        6 * 0.020       !
! ETHE         =       6 * 0.020 ,         6 * 0.040 ,        6 * 0.060       !
! OLE1         =       6 * 0.030 ,         6 * 0.060 ,        6 * 0.080       !
! SO2          =       6 * 0.005 ,         6 * 0.010 ,        6 * 0.020       !
!END!
```

Unformatted BCON.DAT File - Header Records

The header records of the unformatted BCON.DAT file contain information describing the horizontal and vertical grid Systems used in the data base, beginning and ending dates and time of the data in the file, and a list of species. The following parameters stored in the header records are checked In the setup phase of the CALGRID model run in order to ensure compatibility with variables specified in the CALGRID control file: horizontal grid type, vertical grid type, number of grid cells in the X and Y directions, number of vertical layers, grid size, grid origin coordinates, I'm zone of the grid origin. number of species, species names and species ordering. Any mismatch results in an error message and termination of the CALGRID run.

Sample Fortran read statements for the header records are:

```
   READ(iunit) FNAMEB,IGTYPB,IVTYPB,NXB,NYB,NZB,DELXB,DELYB,XORIGB,
  1 YORIGB,IUTMZB,NSAB,IBDATB,IBTIMB,IEDATB,IETIMB,VRSB,LABELB

   READ(iunit)CSLSTB
```

where the following declarations apply:

```
   CHARACTER*12 FNAMEB,VRSB,LABELB,CSLSTB(nsab)
```

Unformatted BCON.DAT File - Data Records

The unformatted `BCON.DAT` file contains a set of "NSA $*$ NZ $+$ 1" records for each time period of data within the file (NSA is the number of advected species and NZ is the number of vertical layers). The first record of each set defines the time period over which the boundary conditions in the following records are valid. This can be a one hour period or any integer multiple number of hours. The next "NSA $*$ NZ" records contain the boundary condition values, in ppm, for each boundary cell as a function of species and vertical layer.

Sample Fortran read statements for the data records are:

```
Loop over time periods (e.g. hours)

   READ(iunit)IBDAT,IBTIM,IEDAT,IETIM

      Loop over species

         Loop over vertical layers

            READ(iunit)CLAB,XBCTOP,XBCBOT,XCLEFT,YBCRIGHT

         End loop over vertical layers

      End loop over species

End loop over time periods
```

where the following declarations apply:

```
character*12 CLAB
real XBCTOP(nxb), XBCBOT(nxb), YBCLEFT(nyb-2),YBCRIGHT(nyb-2)
```

Unformatted BCON.DAT File - Header Record 1 - General Data

NO.	VARIABLE	TYPE[a]	DESCRIPTION	SAMPLE VALUES
1	FNAMEB	C*12	Data set name	BCON
2	IGTYPB	I	Horizontal grid type	1
3	IVTYPB	I	Vertical grid type	2
4	NXB	I	Number of grid cells in the X direction	30
5	NYB	I	Number of grid cells in the Y direction	30
6	NZB	I	Number of vertical layers	5
7	DELXB	R	Grid spacing (km) in the X direction	5.
8	DELYB	R	Grid spacing (km) in the Y direction	5.
9	XORIGB	R	Reference X UTM coordinate (km) of the southwest corner of grid cell (1,1)	168.000
10	YORIGB	R	Reference Y UTM coordinate (km) of the southwest corner of grid cell (1,1)	3839.000
11	IUTMZB	I	UTM zone of horizontal coordinates	11
12	NSEB	I	Number of advected species	36
13	IBDATB	I	Date of beginning of data in file (YYJJJ, where YY=year, JJJ=Julian day)	84220
14	IBTIMB	I	Hour of beginning of data in file (00-23, LST)	00
15	IEDATB	I	Date of ending of data in file (YYJJJ, where YY=year, JJJ=Julian day)	84224
16	IETIMB	I	Hour of ending of data in file (00-23, LST)	23
17	VRSB	C*12	Data set version	Base Case
18	LABELB	C*12	Data set label	’84 -KERN

[a]C*12 = Character*12
I = Integer
R = Real

Unformatted BCON.DAT File - Header Record 2 - Species List

NO.*	TYPE[a]	DESCRIPTION	SAMPLE VALUES
1	C*12	Species identifier for species 1	CO2
2	C*12	Species identifier for species 2	HO2H
3	C*12	Species identifier for species 3	RO2-HO2-PROD
.	.	.	.
.	.	.	.
.	.	.	.
NSAB	C*12	Species identifier for species "NSAB"	SO2

*"NSAB" elements of CSLSTB array

[a]C*12 = Character*12
I = Integer
R = Real

Unformatted BCON.DAT File - Data Record Contents
(Record 1 of each set)

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	IBDAT	I	Beginning date for which data in this set is valid (YYJJJ, where YY=year, JJJ=Julian day)
2	IBTIM	I	Beginning time for which data in this set is valid (00-23) LST
3	IEDAT	I	Ending date for which data in this set is valid (YYJJJ, where YY=year, JJJ=Julian day)
4	IETIM	I	Ending time for which data in this set is valid (00-23) LST

Example:

Data Valid for 1 hour:

IBDAT=89183,IBTIM=00,IEDAT=89183,IETIM=00
IBDAT=89183,IBTIM=01,IEDAT=89183,IETIM=01
IBDAT=89183,IBTIM=02,IEDAT=89183,IETIM=02

Data Valid for 3 hour:

IBDAT=89183,IBTIM=00,IEDAT=89183,IETIM=02
IBDAT=89183,IBTIM=03,IEDAT=89183,IETIM=05
IBDAT=89183,IBTIM=06,IEDAT=89183,IETIM=08

[a]I = Integer

Unformatted BCON.DAT File - Data Record Contents
(Record 2, 3, . . . "NSAB*NSB+1" of each set)

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	CLAB	C*12	Species identifier (up to 12 characters)
Next NXB	XBCTUP	R array	Boundary concentrations (ppm) for the top row of grid cells (X=1 to NX, Y=NY)
Next NXB	XBCBDT	R array	Boundary concentrations (ppm) for the bottom row of grid cells (X=1 to NX, Y=NY)
Next NYB - 2	TBCLEFT	R array	Boundary concentrations (ppm) for the left column of grid cells (X=1, Y=2 to NY-1)
Next NYB - 2	TBCRIGHT	R array	Boundary concentrations (ppm) for the right column of grid cells (X=1, Y=2 to NY-1)

[a]C*12 = Character*12
R = Real

4.1.5 Top Boundary Condition Data File (TCON.DAT)

The TCON.DAT data file contains boundary conditions for each advected species at the top of the modeling domain. Three options, controlled by the control file variable ITTCON, are provided for the input of the top boundary conditions.

ITTCON = 1	for a formatted input file containing one time-independent top boundary condition for each species. There is no spatial variability in the top boundary conditions with this option.
ITTCON = 2	for an unformatted file containing a full 2-D field of time-dependent top boundary conditions for each species. Each top boundary cell can have a different value for each time step with this option.
ITTCON = 3	if the TCON.DAT file is not used. The top boundary conditions are taken from the top layer of the initial concentration field. With this option, the top boundary conditions are time-independent. If the top layer of the initial concentration field has spatial variability (e.g., with ITICON = 2 (see Section 4.1.3)), this will be reproduced in the top boundary condition field.

Formatted Top Boundary Condition File

The formatted top boundary condition file (ITTCON=1) contains one value of the top boundary condition for each advected species. CALGRID internally assigns this value to each of the NX * NY top boundary grid cells. The boundary conditions are specified in units of ppm.

An example of a formatted TCON.DAT data file is shown in Table 4.1.5. The formatted TCON file uses a control file format (see Section 4.1.1). All text outside the delimiters is considered as user comment information and is echoed back but otherwise ignored by the input module. Each data line consists of a delimiter followed by a species name (e.g. O3, SO2. etc.), the top boundary concentration, and a terminating delimiter. The file must end with an input group terminator (i.e., !END!).

The model checks that values have been entered for every advected species in the run. Missing value will result in an error message and termination of the run. The species names must match those used in the chemical mechanism implemented in the model.

Unformatted Top Boundary Condition File

The unformatted top boundary condition file allows the user to specify a full 2-D field of time-dependent boundary condition values for species. The control file variable, `ITTCON`, must be set equal to 2 in order to flag the use of the unformatted file option.

The unformatted `TCON.DAT` file consists of two header records followed by a set of data records. Each data record set contains a record specifying the time period for which the data is valid, followed by NSA records, each with NX * NY top boundary condition values (NSA is the number of advected species, NX, NY are the number of grid cells in the X and Y directions). The time intervals at which the boundary values are updated can be hourly or any multiple hour period, and can vary from record to record within the file.

Table 4.1.5
Sample formatted top boundary condition file (TCON.DAT)

```
                FORMATTED TOP BOUNDARY CONDITION FILE (TCON)
                -------------------------------------------


SPECIES            Top Boundary Condition (ppm)
 NAME
-------            ------------------------------

BUILD-UP SPECIES

! CO2          =              0.51E-13    !
! HO2H         =              0.23E-13    !
! RO2-HO2-PROD =              0.23E-13    !
! RO2-RO2-PROD =              0.23E-13    !
! -OOH         =              0.23E-13    !
! -C           =              0.23E-13    !
! -N           =              0.23E-13    !
! H2           =              0.11E-11    !
! H2SO4        =              0.23E-13    !

ACTIVE SPECIES
! O3           =              0.47E-13    !
! NO           =              0.60E-06    !
! NO2          =              0.20E-06    !
! NO3          =              0.36E-06    !
! N2O5         =              0.21E-06    !
! HNO3         =              0.36E-13    !
! HONO         =              0.48E-13    !
! HNO4         =              0.29E-13    !
! HO2          =              0.68E-13    !
! CO           =              2.12E-06    !
! RO2.         =              0.23E-13    !
! RCO3.        =              0.30E-13    !
! PAN          =              0.19E-13    !
! HCHO         =              0.65E-06    !
! RNO3         =              0.17E-13    !
! MEK          =              0.35E-06    !
! CCHO         =              0.33E-06    !
! MGLY         =              0.31E-13    !
! CRES         =              0.63E-06    !
! AFG2         =              0.31E-13    !
! AAR1         =              0.12E-06    !
! AAR2         =              0.22E-06    !
! AAR3         =              0.11E-06    !
! AAR4         =              0.63E-06    !
! ETHE         =              0.30E-06    !
! OLE1         =              0.33E-06    !
! SO2          =              0.96E-06    !

!END!
```

Unformatted TCON.DAT File Header Records

The header records of the unformatted TCON.DAT file contain information describing the horizontal grid system used in the data base, beginning and ending dates and time of the data in the file, and a list of species. The following parameters stored in the header records are checked in the setup phase of the CALGRID model run in order to ensure compatibility with variables specified in the CALGRID control file: horizontal grid type, number of grid cells in the X and Y directions, grid size, grid origin coordinates, UTM zone of the grid origin, number of species, species names and species ordering. Any mismatch results in an error message and termination of the CALGRID run.

Sample Fortran read statements for the header records are:

```
 READ(iunit)FNAMET, IGTYPT, NXT, NYT, DELXT, DELYT, XORIGT,
1 Y0RIGT ,IUTMZT, NSAT, IBDATT, IBTIMT, IEDATT, IETIMT, VRST,
2 LABELT

 READ(lunit)CSLSTT
```

where the following declarations apply:

```
CHARACTER*12 FNAMET, VRST, LABELT, CSLSTT(nsat)
```

Unformatted TCON.DAT File - Header Record 1 - General Data

NO.	VARIABLE	TYPE[a]	DESCRIPTION	SAMPLE VALUES
1	FNAMET	C*12	Data set name	TCON
2	IGTYPT	I	Horizontal grid type	1
3	NXT	I	Number of grid cells in the X direction	30
4	NYT	I	Number of grid cells in the Y direction	30
5	DELXT	R	Grid spacing (km) in the X direction	5.
6	DELYT	R	Grid spacing (km) in the Y direction	5.
7	XORIGT	R	Reference X UTM coordinate (km) of the southwest corner of grid cell (1,1)	168.00
8	YORIGT	R	Reference Y UTM coordinate (km) of the southwest corner of grid cell (1,1)	3839.00
9	IUTMZT	I	UTM zone of horizontal coordinates	11
10	NSAT	I	Number of advected species	36
11	IBDATT	I	Date of beginning of data in file (YYJJJ, where YY=year, JJJ=Julian day)	84220
12	IBTIMT	I	Hour of beginning of data in file (00-23, LST)	00
13	IEDATT	I	Date of ending of data in file (YYJJJ, where YY=year, JJJ=Julian day)	84220
14	IETIMT	I	Hour of ending of data in file (00-23, LST)	23
15	VRST	C*12	Data set version	Base Case
16	LABELT	C*12	Data set label	’84 - KERN

[a]C*12 = Character*12
I = Integer
R = Real

Unformatted TCON.DAT File - Header Record 2 - Species List

NO.*	TYPE[a]	DESCRIPTION	SAMPLE VALUES
1	C*12	Species identifier for species 1	CO2
2	C*12	Species identifier for species 2	HO2H
3	C*12	Species identifier for species 3	RO2-HO2-PROD
.	.	.	.
.	.	.	.
.	.	.	.
NSAT	C*12	Species identifier for species "NSAT"	SO2

*"NSAT" elements of CSLSTT array
[a]C*12 = Character*12

Unformatted TCON.DAT **File - Data Records**

The unformatted TCON.DAT file contains a set of "NSA + 1" records for each time period of data within the file (NSA is the number of advected species). The first record of each set defines the time period over which the boundary conditions in the following records are valid. This can be a one hour period or any integer multiple number of hours. The next "NSA" records contain the boundary condition values, in ppm, for each boundary cell as a function of species.

Sample Fortran read statements for the data records are:

```
Loop over time periods (e.g. hours)

   READ(iunit)IBDAT,IBTIM,IEDAT,IETIM

      Loop over species

         READ ( lunit )CLAB, XTBC

      End loop over species

End loop over time periods
```

where the following declarations apply:

```
character*12 CLAB
real XTBC(nxt,nyt)
```

Unformatted TCON.DAT File - Data Record Contents
(Record 1 of each set)

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	IBDAT	I	Beginning date for which data in this set is valid (YYJJJ, where YY=year, JJJ=Julian day)
2	IBTIM	I	Beginning time for which data in this set is valid (00-23, LST)
3	IEDAT	I	Ending date for which data in this set is valid (YYJJJ, where YY=year, JJJ=Julian day)
4	IETIM	I	Beginning time for which data in this set is valid (00-23, LST)

Example:

Data Valid for 1 hour:

IBDAT=89183,IBTIM=00,IEDAT=89183,IETIM=00
IBDAT=89183,IBTIM=01,IEDAT=89183,IETIM=01
IBDAT=89183,IBTIM=02,IEDAT=89183,IETIM=02

Data Valid for 3 hour:

IBDAT=89183,IBTIM=00,IEDAT=89183,IETIM=02
IBDAT=89183,IBTIM=03,IEDAT=89183,IETIM=05
IBDAT=89183,IBTIM=06,IEDAT=89183,IETIM=08

[a] I = Integer

Unformatted TCON.DAT File - Data Record Contents
(Record 2, 3, . . . "NSAT+1" of each set)

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	CLAB	C*12	Species identifier (up to 12 characters)
Next NXT*NYT	XTBC	R array	Top boundary concentrations (ppm) for each grid cell

[a]C*12 = Character*12
R = Real

4.1.6 Point Source Emissions File #1 - Cyclical or Constant Emissions (PTEMCYC.DAT)

The PTEMCYC.DAT emissions file contains point source emissions data for stationary sources with characteristics which do not vary or vary according to diurnal and/or day of week cycles. The emissions data for stationary sources with arbitrarily varying emission parameters that cannot be described by the day of week and diurnal variation factors are contained in a separate, optional file (FTEMARB.DAT). A third point source file (PTEMMOB.DAT) contains the emissions data for mobile point sources, such as ships. With these files, the plume rise computations are performed internally within the CALGRID model.

The PTEMCYC.DAT file consists of eight header records describing the exact format of the file followed by a set of data records. The file is a direct-access file to allow repeated reading of the data records. There is one data record for each point source. The header records allow flexibility in the construction of the inventory. For example, the inventory may include day of week and/or diurnal variation factors in the emission rates and stack. parameters, or unvarying, averaged values only, without cycles. The number of day of week categories and diurnal categories are specified in the header records. The diurnal and day of week factors can be different for each point source in the PTEMCYC.DAT file. However, each record in the inventory must be of the same format.

Each point source data record contains a set a 10 parameters describing the source location, type, elevation, stack characteristics and averaged emission rates. In addition, each point source record may contain day of week and diurnal factors describing variations in emission parameters (i.e., emission rate, temperature, and flow rate). The emission parameters for a given hour are related to the averaged values by:

$$Q_S = \overline{Q}_S * (\text{Day of week factor})_{i,s1} * (\text{Diurnal factor})_{j,k,s2} \quad (1)$$

$$T = \overline{T} * (\text{Day of week factor})_{i} * (\text{Diurnal factor})_{j,k} \quad (2)$$

$$V = \overline{V} * (\text{Day of week factor})_{i} * (\text{Diurnal factor})_{j,k} \quad (3)$$

where

$\overline{Q}_S$, $\overline{T}$, and $\overline{V}$ are the averaged emission rate (g/s), temperature (deg. K), and flow rate (m^3/s), and,
Q_S, T, and V are the actual emission rate (g/s), temperature (deg. K), and flow rate (m^3/s),

and the subscripts are defined as:

- s is the species,
- $s1$ is the species category for the day of week scaling (e.g., if three species groups are used, one possible scheme is for $s1 = 1$ for NO_x, $s1 = 2$ for all HC species, $s1 = 3$ for SO_2).
- $s2$ is the species category for the diurnal scaling (e.g., $s2 = 1$ for NO_x, $s2 = 2$ for CO, $s2 = 3$ for HC species, $s2 = 4$ for SO_x). Note: the species groups for the diurnal scaling need not be the same as those for the day of week scaling.
- i is the day of week category (e.g., if two day of week categories are used, one possibility is $i = 1$ for weekdays, $i = 2$ for weekends).
- j is the hour index (e.g., $j = 1$ for hours 00-03, $j = 2$ for hours 03-06, $j = 3$ for 06-09, etc.).
- k is the day of week category for the diurnal factors (e.g., 2 groups of diurnal factors would allow separate sets of djurnal factors for weekends and weekdays).

If the emission parameters do not vary as a function of time for any of the sources in the file, the data file becomes very simple. Under these conditions, there is only one diurnal category for all hours and one day of week factor for all days. The diurnal and day of week factors should be set to unity, so that the averaged values of the emission rates and stack parameters will always be used.

The CALGRID model contains cross-referencing arrays so that the point sources need not be in any particular order. There is no limit on the number of point sources allowed. This file is designed to be independent of the horizontal arid vertical grid system being used in the model. The grid cell location of each source is determined from its UTM coordinates. Hourly plume rise for each point source is computed within the model, and the emissions are assigned to the appropriate vertical layer or layers based on the effective plume height.

The maximum record length of the direct-access file is specified in the Fortran open statement. The maximum record length must be sized to accomodate the longest of the data or header records. The maximum length, in words, of each record of the direct-access file is the maximum of:

$3 * \text{NSEl}$

$24,$ or,

$14 + \text{NSE1} + \text{NWKCAT} * (\text{NWKADJ} + 2) + \text{NDI} * (\text{NDIADJ} + 2) * \text{NDICAT}$

PTEMCYC.DAT **File Header Records**

The eight header records of the PTEMCYC.DAT file contain information describing the contents and format of the data records. They include a list of the emitted species, molecular weights, definitions of the diurnal and day of week emission adjustment categories and variation factors. Sample read statements for the header records are:

```
 READ(iunit,REC=1)FNAME1,NSRC1,NSE1,NWKCAT,NWKADJ,NDICAT,NDIADJ,
1 MDI, IUTMZ1,VRS1,LABEL1
 READ(iunit,REC=2)CSLST1
 READ(iunit,REC=3)XMWEM1
 READ(iunit,REC=4)IDOWSS
 READ(iunit,REC=5)IDOWDI
 READ(iunit,REC=6)IHRDI
 READ(iunit,REC=7)ISPDOW
 READ(iunit,REC=8)ISPDI
```

where the following declarations apply:

```
CHARACTER*12 FNAME1,VRS1,LABEL1 CSLST1(nse1)
REAL XMWEM1(nsel)
INTEGER IDOWSS(7),IDOWDI(7),IHRDI(24)
INTEGER ISPDOW(nse1),ISPDI(nse1)
```

The contents of each record are described below.

PTEMCYC.DAT - Header Record 1 - General Format Data

NO.	VARIABLE	TYPE	RANGE	DESCRIPTION	SAMPLE* VALUES
1	FNAME1	C*12	-	Data set name	PTEMCYC
2	NSRC1	I	≥ 1	Number of point sources in file	2000
3	NSE1	I	≥ 1	Number of species emitted	13
4	NWKCAT	I	≥ 1	Number of day of week categories	2
5	NWKADJ	I	≥ 1	Number of species groups in each day of week category	3
6	NDICAT	I	≥ 1	Number of diurnal adjustment categories per week	1
7	NDIADJ	I	≥ 1	Number of species groups in each diurnal adjustment category	4
8	NDI	I	≥ 1	Number of diurnal adjustment factors in each day	8
9	IUTMZ1	I	-	UTM zone in which stack coordinates are specified	11
10	VRS1	C*12	-	Data set version	Base Case
11	LABEL1	C*12	-	Data set label	'84 - KERN

*

NSRC1	=	2000	indicates the number of point sources included in the PTEMCYC file
NSE1	=	13	indicates thirteen species are emitted (e.g., NO, NO_2, CO, HCHO, MEK, CCHO, AAR1, AAR2, AAR3, MR4, ETHE, OLEl, SO_2)
NWKCAT	=	2	for two day of week adjustment categories (e.g., weekdays and weekends)
NWKADJ	=	3	for three day of week species groups (e.g., SO_2 adjusted with one set of day of week factors, NO_X with another, and all other species with a third set of factors)
NDICAT	=	1	indicates the same set of diurnal factors are used for both day of week categories (i.e., weekend and weekdays)
NDIADJ	=	4	for four diurnal species groups (e.g., NO_X, CO, HC species, SO_2)
NDI	=	8	indicates that eight diurnal categories are used (e.g., Hours 00-03, 03-06, 06-09, 9-12, 12-15, 15-18, 18-21, 21-24)

PTEMCYC.DAT - Header Record 2 - Species List

NO.*	TYPE[a]	DESCRIPTION	SAMPLE VALUES
1	C*12	Species identifier for species 1	NO
2	C*12	Species identifier for species 2	NO2
3	C*12	Species identifier for species 3	CO
.	.	.	.
.	.	.	.
.	.	.	.
NSE1	C*12	Species identifier for species “NSE1”	SO2

* “NSE1” elements of CSLST1 array

[a] C*12 = Character*12

PTEMCYC.DAT - Header Record 3 - Molecular Weights

NO.*	TYPE[a]	DESCRIPTION	SAMPLE VALUES
1	R	Molecular weight for species 1	30.01 (NO)
2	R	Molecular weight for species 2	46.01 (NO2)
3	R	Molecular weight for species 3	28.01 (CO)
.	.	.	.
.	.	.	.
.	.	.	.
NSE1	R	Molecular weight for species "NSE1"	64.07 (SO2)

* "NSE1" elements of SMWEM1 array

[a] R = Real

PTEMCYC.DAT - Header Record 4 - Mapping of Days to Day of Week Categories

NO.*	TYPE[a]	RANGE	DESCRIPTION	SAMPLE** VALUES
1	I	1 – NWKCAT	Day of week category to which Sunday is assigned.	2
2	I	1 – NWKCAT	Day of week category to which Monday is assigned.	1
3	I	1 – NWKCAT	Day of week category to which Tuesday is assigned.	1
4	I	1 – NWKCAT	Day of week category to which Wednesday is assigned.	1
5	I	1 – NWKCAT	Day of week category to which Thursday is assigned.	1
6	I	1 – NWKCAT	Day of week category to which Friday is assigned.	1
7	I	1 – NWKCAT	Day of week category to which Saturday is assigned.	2

* 7 elements of IDOWSS array

** Sample shows two day of week categories: weekends and weekdays.

a I = Integer

PTEMCYC.DAT - Header Record 5 - Mapping of Days to Diurnal Categories

NO.*	TYPE[a]	RANGE	DESCRIPTION	SAMPLE** VALUES
1	I	1 – NDICAT	Diurnal category to which Sunday is assigned.	1
2	I	1 – NDICAT	Diurnal category to which Monday is assigned.	1
3	I	1 – NDICAT	Diurnal category to which Tuesday is assigned.	1
4	I	1 – NDICAT	Diurnal category to which Wednesday is assigned.	1
5	I	1 – NDICAT	Diurnal category to which Thursday is assigned.	1
6	I	1 – NDICAT	Diurnal category to which Friday is assigned.	1
7	I	1 – NDICAT	Diurnal category to which Saturday is assigned.	1

* 7 elements of IDOWDI array

** Sample shows that one diurnal cycle is applied for all days.

[a] I = Integer

PTEMCYC.DAT - Header Record 6 - Mapping of Hours to Diurnal Categories

NO.*	TYPE[a]	RANGE	DESCRIPTION	SAMPLE** VALUES
1	I	1 – NDI	Diurnal category to which Hour 00-01 is assigned.	1
2	I	1 – NDI	Diurnal category to which Hour 01-02 is assigned.	1
3	I	1 – NDI	Diurnal category to which Hour 02-03 is assigned.	1
4	I	1 – NDI	Diurnal category to which Hour 03-04 is assigned.	2
5	I	1 – NDI	Diurnal category to which Hour 04-05 is assigned.	2
6	I	1 – NDI	Diurnal category to which Hour 05-06 is assigned.	2
7	I	1 – NDI	Diurnal category to which Hour 06-07 is assigned.	3
.	.	.	.	.
.	.	.	.	.
.	.	.	.	.
24	I	1 – NDI	Diurnal category to which Hour 23-24 is assigned.	8

* 24 elements of IHRDI array

** For example, with NDI=8, and IHRDI = 1,1,1,2,2,2,3,3,3,4,4,4,5,5,5, 6,6,6,7,7,7,8,8,8 indicates emission factors are provided 8 times per day in three hour increments (Hours 00-03, 03-06, 06-09, etc.)

[a] I = Integer

PTEMCYC.DAT - Header Record 7 - Mapping of Species to Day of Week Categories

NO.*	TYPE[a]	RANGE	DESCRIPTION	SAMPLE** VALUES
1	I	1 – NWKADJ	Day of week category to which Species 1 is assigned.	1
2	I	1 – NWKADJ	Day of week category to which Species 2 is assigned.	1
3	I	1 – NWKADJ	Day of week category to which Species 3 is assigned.	1
4	I	1 – NWKADJ	Day of week category to which Species 4 is assigned.	2
5	I	1 – NWKADJ	Day of week category to which Species 5 is assigned.	2
.	.	.	.	.
.	.	.	.	.
.	.	.	.	.
NSE1	I	1 – NWKADJ	Day of week category to which Species "NSE1" is assigned.	3

* "NSE1" elements of ISPDOW array

** For example, using species in Header Record 2, and with ISPDOW = 1,1,2,2,2,2,2,2,2,2,2,2,3, three day of week cycles are used for different species: NO, NO2, use one day of week cycle, CO, HCHO, MEK, CCHO, AARl, AAR2, AAR3, AAR4, ETHE, OLEl use the second cycle, and SO2 uses the third cycle.

[a] I = Integer

PTEMCYC.DAT - Header Record 8 - Mapping of Species to Diurnal Categories

NO.*	TYPE[a]	RANGE	DESCRIPTION	SAMPLE** VALUES
1	I	1 – NDIADJ	Diurnal category to which Species 1 is assigned.	1
2	I	1 – NDIADJ	Diurnal category to which Species 2 is assigned.	1
3	I	1 – NDIADJ	Diurnal category to which Species 3 is assigned.	2
4	I	1 – NDIADJ	Diurnal category to which Species 4 is assigned.	3
5	I	1 – NDIADJ	Diurnal category to which Species 5 is assigned.	3
.	.	.	.	.
.	.	.	.	.
.	.	.	.	.
NSE1	I	1 – NDIADJ	Diurnal category to which Species "NSE1" is assigned.	4

* "NSE1" elements of ISPDI array

** For example, using species in Header Record 2, and with ISPDI = 1,1, 2, 3, 3, 3, 3, 3, 3, 3, 3, 3, 4, four diurnal cycles are used for different species: NO, NO2, use one diurnal cycle, CO uses the second diurnal cycle, HCHO, MEK, CCHO, AARl, AAR2, AAR3, AAR4, ETHE, OLE1 use the third cycle, and SO2 uses the four cycle.

[a] I = Integer

PTEMCYC.DAT **File - Data Records**

The PTEMCYC.DAT data file contains one data record for each point source. The data records begin at Record 9. With the 8 header records, the total number of records in the file is 8+NSRCl, where NSRC1 is the number of sources.

A sample Fortran read statement for a PTEMCYC.DAT data record is:

```
Loop over sources

READ(iunit,REC=nrec)CID,SDATA,QAVE,QFDOW,SFDOW,QFDI,SFDI

End loop over sources
```

where the following declarations apply:

```
CHARACTER*16 CID
REAL SDATA(10),QAVE(nsel)
REAL QFDOW(nwkcat,nwkadj),SFDOW(nwkcat,2)
REAL QFDI(ndi,ndiadj,ndicat),SFDI(ndi,2,ndicat)
```

The definition of each of these variables is described in detail below.

PTEMCYC.DAT - Data Record Contents

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	CID	C*16	Source identifier (16 characters=4 words)
2	SDATA(1)	R	Easting UTM coordinate (km) of source
3	SDATA(2)	R	Northing UTM coordinate (km) of source
4	SDATA(3)	R	Stack height (m)
5	SDATA(4)	R	Stack diameter (m)
6	SDATA(5)	R	Average exit temperature (deg. K)
7	SDATA(6)	R	Average exit velocity (m/s)
8	SDATA(7)	R	Average volumetric flow rate (m^3/s)
9	SDATA(8)	R	Stack base elevation (m)
10	SDATA(9)	R	User defined flag (e.g., industry code)
11	SDATA(10)	R	User defined flag (e.g., fuel code)
Next NSE1	QAVE	R Array	Average emission rate (g/s) for each species in the order specified in Header Record 2
Next (NWKCAT * NWKADJ)	QFDOW	R Array	Day of week emission rate adjustment factors for species groups 1 to NWKADJ (QFDOW(nwkcat,nwkadj))
Next (NWKCAT * 2)	SFDOW	R Array	Day of week adjustment factors for exit temperature and exit velocity (SFDOW(nwkcat,2))[b]
Next (NDI * NDIADJ * NDICAT)	QFDI	R Array	Diurnal emission factors for species groups 1 to NDIADJ (QFDI(ndi,ndiadj,ndicat))
Next (NDI * 2 * NDICAT)	SFDI	R Array	Diurnal adjustment factors for exit temperature and exit velocity (SFDI(ndi,2,ndicat))[b]

[a] C*16 = Character*16
R = Real

[b] The dimension of 2 in the SFDOW and SFDI arrays corresponds to the factors for exit temperature (Location 1) and exit velocity (Location 2).

4.1.7 Point Source Emissions File #2 - Arbitrarily Varying Emissions (PTEMARB.DAT)

The PTEMARB.DAT file contains point source emissions data for sources with detailed, arbitrarily varying emissions parameters that cannot be described by the day of week and diurnal factors used in the regular point source file (PTEMCYC.DAT). In the PTEMARB.DAT file, values for the stack parameters and emission rates can be specified for each time step in the run. Plume rise is computed within the CALGRID model for each source.

PTEMARB.DAT is a sequential, unformatted data file consisting of three header records, followed by a set of data records containing time-invariant source information. The time-invariant records contain the stack height, diameter, coordinates, and optional descriptive codes for each source. The time varying emissions and stack parameter data follow in subsequent records. One data record per source is required for each time period (e.g.,usually at hourly intervals).

The data in the PTEMARB.DAT file is independent of the horizontal and vertical grid systems being used in the model. The horizontal coordinates are specified in terms of UTM coordinates. The vertical layers receiving the emissions of the source are based on the plume rise of the source computed internally by the model. However, the PTEMARB.DAT file does contain time-dependent data specifying the emission parameters for a particular time period.

PTEMARB.DAT File - Header Records

The header records of the PTEMARB.DAT file contain the number of sources, starting and ending time periods of data in the file, and a list of the emitted species. Sample Fortran read statements are:

```
      READ(iunit)FNAME2,NSRC2,NSE2,IUTMZ2,IBDAT2,IBTIM2,IEDAT2,
     1 IETIM2,VRS2,LABEL2


      READ(iunit)CSLST2
      READ(iunit)XMWEM2
```

where the following declarations apply:

```
      CHARACTER*12 FNAME2,VRS2,LABEL2,CSLST2(nse2)
      REAL XMWEM2(nse2)
```

PTEMARB.DAT - Header Record 1 - General Data

NO.	VARIABLE	TYPE[a]	DESCRIPTION	SAMPLE VALUES
1	FNAME2	C*12	Data set name	PTEMARB
2	NSRC2	I	Number of point sources in file	10
3	NSE2	I	Number of species emitted	13
4	IUTMZ2	I	UTM zone in which source coordinates are specified	11
5	IBDAT2	I	Date of beginning of data i the file (YYJJJ, where YY=year, JJJ=Julian day)	84220
6	IBTIM2	I	Hour of begining of data in the file (00-23, LST)	00
7	IEDAT2	I	Date of ending of data i the file (YYJJJ, where YY=year, JJJ=Julian day)	84224
8	IETIM2	I	Hour of ending of data in the file (00-23, LST)	23
9	VRS2	C*12	Data set version	Base Case
10	LABEL2	C*12	Data set label	Major pts.

[a] C*12 = Character*12
I = Integer

PTEMARB.DAT - Header Record 2 - Species List

NO.*	TYPE[a]	DESCRIPTION	SAMPLE VALUES
1	C*12	Species identifier for species 1	NO
2	C*12	Species identifier for species 3	NO2
3	C*12	Species identifier for species 3	CO
.	.	.	.
.	.	.	.
.	.	.	.
NSE2	C*12	Species identifier for species “NSE2”	SO2

* “NSE2” elements of CSLST2 array

[a] C*12 = Character*12

PTEMARB.DAT - Header Record 3 - Molecular Weights

NO.*	TYPE[a]	DESCRIPTION	SAMPLE VALUES
1	R	Molecular weight for species 1	30.01 (NO)
2	R	Molecular weight for species 3	46.01 (NO2)
3	R	Molecular weight for species 3	28.01 (CO)
.	.	.	.
.	.	.	.
.	.	.	.
NSE2	R	Molecular weight for species "NSE2"	64.07 (SO2)

* "NSE2" elements of XMWEM2 array

[a] R = Real

PTEMARB.DAT File - Data Records

The PTEMARB.DAT file contains two types of data records. A set of time-invariant records are read after the header records. These records specify the time-invariant source parameters, including the source coordinates, stack height, and diameter. A set of time-varying data follows. The time-varying records contain the stack temperature, exit velocity, flow rate, and emission rate for each species.

Sample Fortran read statements for time-invariant data records are:

```
Loop over sources

READ(iunit)CID,TIDATA

End loop over sources
```

where the following declarations apply:

```
CHARACTER*16 CID
REAL TIDATA(7)
```

Sample Fortran read statements for time-varying data records are:

```
Loop over time periods

READ(iunit)IBDAT,IBTIM,IEDAT,IETIM

    Loop over sources

    READ(iunit)CID,TEMPK,VEXIT,VOLFLOW,QEMIT

    End loop over sources

End loop over time periods
```

where the following declarations apply:

```
CHARACTER*16 CID
REAL QEMIT(nse2)
```

PTEMARB.DAT - Time-Invariant Data Record Contents
(Repeated for each source)

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	CID	C*16	Source identifier (16 characters=4 words)
2	TIDATA(1)	R	Easting UTM coordinate (km) of the source
3	TIDATA(2)	R	Northing UTM coordinate (km) of the source
4	TIDATA(3)	R	Stack height (m)
5	TIDATA(4)	R	Stack diameter (m)
6	TIDATA(5)	R	Stack base elevation (m)
7	TIDATA(6)	R	User defined flag (e.g., industry code)
8	TIDATA(7)	R	User defined flag (e.g., fuel code)

[a] C*16 = Character*16
R = Real

PTEMARB.DAT - Time-Varying Data Record Contents
(First record of "NSRC2"+1 records required for each time period)

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	IBDAT	I	Beginning date for which data in this set is valid (YYJJJ, where YY=year, JJJ=Julian day)
2	IBTIM	I	Beginning time for which data in this set is valid (00-23) LST
3	IEDAT	I	Ending date for which data in this set is valid (YYJJJ, where YY=year, JJJ=Julian day)
4	IETIM	I	Ending time for which data in this set is valid (00-23) LST

Example:

Data Valid for 1 hour:

IBDAT=89183,IBTIM=00,IEDAT=89183,IETIM=00
IBDAT=89183,IBTIM=01,IEDAT=89183,IETIM=01
IBDAT=89183,IBTIM=02,IEDAT=89183,IETIM=02

Data Valid for 3 hour:

IBDAT=89183,IBTIM=00,IEDAT=89183,IETIM=02
IBDAT=89183,IBTIM=03,IEDAT=89183,IETIM=05
IBDAT=89183,IBTIM=06,IEDAT=89183,IETIM=08

[a]I = Integer

PTEMARB.DAT - Time-Varying Data Record Contents
(Next "NSRC2" records)

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	CID	C*16	Source identifier (must match values in time-invariant records)
2	TEMPK	R	Exit temperature (deg. K)
3	VEXIT	R	Exit velocity (m/s)
4	VOLFLOW	R	Volumetric flow rate (m^3/s)
Next NSE1	QEMIT	R array	Emission rates (g/s) for each species in the order specified in Header Record 2

[a]C*16 = Character*16
R = Real

4.1.8 Point Source Emissions File #3 - Mobile Point Sources (PTEMMOB.DAT)

The PTEMMOB.DAT file contains point source emissions data for mobile sources, such as ships, with emission rates and source characteristics which do not vary with time. The location of the source is allowed to vary hourly. Plume rise for these sources is computed by the CALGRID model.

The PTEMMOB.DAT file is a sequential, unformatted data file consisting of three header records, followed by a set of time-invariant data records. The time-invariant records contain the stack height, diameter, flow rate, and emission rates of each source. Following the time-invariant data is time varying source location information. The time varying data consists of two records per time period containing the UTM coordinates of each source.

The PTEMMOB.DAT file is independent of the horizontal and vertical grid systems being used in the model. The horizontal coordinates in the file are specified in terms of UTM coordinates. The vertical layers receiving the emissions of the source are based on the plume rise of the source computed internally by the model. However the file does contain time-dependent data describing the average location of each source during each time step.

PTEMMOB - Header Records

The header records of the PTEMMOB file contain specifications of the number of sources, starting and ending time periods, and a list of the emitted species. Sample Fortran read statements are:

```
 READ(iunit)FNAME3,NSRC3,NSE3,IUTMZ3,IBDAT3,IBTIM3,IEDAT3,
1 IETIM3,VRS3,LABEL3


 READ(iunit)CSLST3
 READ(iunit)XMWEM3
```

where the following declarations apply:

```
CHARACTER*12 FNAME3,VRS3,LABEL3,CSLST3(nse3)
REAL XMWEM3(nse3)
```

PTEMMOB.DAT - Header Record 1 - General Data

NO.	VARIABLE	TYPE[a]	DESCRIPTION	SAMPLE VALUES
1	FNAME3	C*12	Data set name	PTEMMOB
2	NSRC3	I	Number of sources in file	30
3	NSE3	I	Number of species emitted	13
4	IUTMZ3	I	UTM zone in which source coordinates are specified	11
5	IBDAT3	I	Date of beginning of data i the file (YYJJJ, where YY=year, JJJ=Julian day)	84220
6	IBTIM3	I	Hour of begining of data in the file (00-23, LST)	00
7	IEDAT3	I	Date of ending of data i the file (YYJJJ, where YY=year, JJJ=Julian day)	84224
8	IETIM3	I	Hour of ending of data in the file (00-23, LST)	23
9	VRS3	C*12	Data set version	Base Case
10	LABEL3	C*12	Data set label	Ship data

[a] C*12 = Character*12
I = Integer

PTEMMOB.DAT - Header Record 2 - Species List

NO.*	TYPE[a]	DESCRIPTION	SAMPLE VALUES
1	C*12	Species identifier for species 1	NO
2	C*12	Species identifier for species 3	NO2
3	C*12	Species identifier for species 3	CO
.	.	.	.
.	.	.	.
.	.	.	.
NSE3	C*12	Species identifier for species “NSE3”	SO2

* “NSE3” elements of CSLST3 array

[a] C*12 = Character*12

PTEMMOB.DAT - Header Record 3 - Molecular Weights

NO.*	TYPE[a]	DESCRIPTION	SAMPLE VALUES
1	R	Molecular weight for species 1	30.01 (NO)
2	R	Molecular weight for species 3	46.01 (NO2)
3	R	Molecular weight for species 3	28.01 (CO)
.	.	.	.
.	.	.	.
.	.	.	.
NSE3	R	Molecular weight for species "NSE3"	64.07 (SO2)

* "NSE3" elements of XMWEM3 array

[a] R = Real

PTEMMOB.DAT File - Data Records

The PTEMMOB.DAT file contains two types of data records. A set of time-invariant records are read after the header records. The time-invariant records specify the source parameters, including the source height, diameter, flow rate, and emission rates for each species. A set of time-varying data follows. The time-varying records contain the average UTM coordinates for each source for each time period.

Sample Fortran read statements for time-invariant data records are:

```
Loop over sources

READ(iunit)CID,XDATA,QEMIT

End loop over sources
```

where the following declarations apply:

```
CHARACTER*16 CID
REAL XDATA(8),QEMIT(nse3)
```

Sample Fortran read statements for time-varying data records are:

```
Loop over time periods

READ(iunit)IBDAT,IBTIM,IEDAT,IETIM
READ(iunit)XUTM
READ(iunit)YUTM

End loop over time periods
```

where the following declarations apply:

```
REAL XUTM(nsrc3),YUTM(nsrc3)
```

PTEMMOB.DAT - Time-Invariant Data Record Contents
(Repeated for each source)

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	CID	C*16	Source identifier (16 characters=4 words)
2	SIDATA(3)	R	Stack height (m)
3	SIDATA(4)	R	Stack diameter (m)
4	SIDATA(1)	R	Average exit temperature (deg. K)
5	SIDATA(2)	R	Average exit velocity (m/s)
6	SIDATA(5)	R	Average volumetric flow rate (m^3/s)
7	SIDATA(6)	R	User defined flag (e.g., source code)
8	SIDATA(7)	R	User defined flag (e.g., industry code)
9	SIDATA(8)	R	User defined flag (e.g., fuel code)
Next NSE3	QEMIT	R array	Emission rates (g/s) for each species in the order specified in Header Record 2

[a] C*16 = Character*16
R = Real

PTEMMOB.DAT - Time-Varying Data Record Contents
(Record 1 of 3 for each time period)

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	IBDAT	I	Beginning date for which data in this set is valid (YYJJJ, where YY=year, JJJ=Julian day)
2	IBTIM	I	Beginning time for which data in this set is valid (00-23) LST
3	IEDAT	I	Ending date for which data in this set is valid (YYJJJ, where YY=year, JJJ=Julian day)
4	IETIM	I	Ending time for which data in this set is valid (00-23) LST

Example:

Data Valid for 1 hour:

IBDAT=89183,IBTIM=00,IEDAT=89183,IETIM=00
IBDAT=89183,IBTIM=01,IEDAT=89183,IETIM=01
IBDAT=89183,IBTIM=02,IEDAT=89183,IETIM=02

Data Valid for 3 hour:

IBDAT=89183,IBTIM=00,IEDAT=89183,IETIM=02
IBDAT=89183,IBTIM=03,IEDAT=89183,IETIM=05
IBDAT=89183,IBTIM=06,IEDAT=89183,IETIM=08

[a]I = Integer

PTEMMOB.DAT - Time-Varying Data Record Contents
(Record 2 of 3 for each time period)

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	XUTM	R array	Easting UTM coordinate (km) of the source for the current time period (XUTM(nsrc3))

(Record 3 of 3 for each time period)

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	YUTM	R array	Northing UTM coordinate (km) of the source for the current time period (YUTM(nsrc3))

[a]R = Real

4.1.9 Area Source Emissions File (AREM.DAT)

The AREM.DAT emissions file contains gridded area source emissions data. It is a sequential, unformatted data file containing one two-dimensional grid for each emitted species modeled by CALGRID for each time step. There are three header records with information describing the grid system, dates and time of data in the file, species names, and molecular weights.

The total emission rate for each pollutant is specified for the grid column. Individual source information is not stored in the file, so plume rise is not computed by CALGRID for the AREM.DAT emissions. However, CALGRID does contain a distribution function which determines the vertical injection of the AREM.DAT emissions. For example, this function controls whether all the area source emissions are injected into the lowest layer or distributed among two or more layers. (See variables NZEM, ZFEM, and WTEM of Input Group 1 in the control file inputs.)

AREM File - Header Records

The header records contain information regarding the horizontal grid system, species emitted, molecular weights, and dates of the data contained in the file. These data are checked by CALGRID in the setup phase of the model run to ensure the parameters are compatible with those specified in the CALGRID control file. Any mismatch in the specifications results in an error message and termination of the run.

Sample Fortran read statements for the header records are:

```
      READ(iunit)FNAME4,IGTYP4,NX4,NY4,DELX4,DELY4,XORIG4,YORIG4,IUTMZ4,
     1 NSE4,IBDAT4,IBTIM4,IEDAT4,IETIM4,VRS4,LABEL4

      READ(iunit)CSLST4
      READ(iunit)XMWEM4
```

where the following declarations apply:

```
      CHARACTER*12 FNAME4,VRS4,LABEL4,CSLST4(nse4)
      REAL XMWEM4(nse4)
```

AREM.DAT - Header Record 1 - General Grid, Species, and Date Data

NO.	VARIABLE	TYPE[a]	DESCRIPTION	SAMPLE VALUES
1	FNAME4	C*12	Data set name	AREM
2	IGTYP4	I	Horizontal grid type	1
3	NX4	I	Number of grid cells in the X direction	30
4	NY4	I	Number of grid cells in the Y direction	30
5	DELX4	I	Grid spacing (km) in the X direction	5.
6	DELY4	I	Grid spacing (km) in the Y direction	5.
7	XORIG4	I	Reference X UTM coordinate (km) of the southwest corner of the gird cell (1,1)	168.0
8	YORIG4	I	Reference Y UTM coordinate (km) of the southwest corner of the gird cell (1,1)	3839.0
9	IUTMZ4	I	UTM zone in which source coordinates are specified	11
10	NSE4	I	Number of species emitted	13
11	IBDAT4	I	Date of beginning of data i the file (YYJJJ, where YY=year, JJJ=Julian day)	84220
12	IBTIM4	I	Hour of begining of data in the file (00-23, LST)	00
13	IEDAT4	I	Date of ending of data i the file (YYJJJ, where YY=year, JJJ=Julian day)	84224
14	IETIM4	I	Hour of ending of data in the file (00-23, LST)	23
15	VRS4	C*12	Data set version	Base Case
16	LABEL4	C*12	Data set label	’84 - KERN

[a] C*12 = Character*12
I = Integer
R = Real

AREM.DAT - Header Record 2 - Species List

NO.*	TYPE[a]	DESCRIPTION	SAMPLE VALUES
1	C*12	Species identifier for species 1	NO
2	C*12	Species identifier for species 3	NO2
3	C*12	Species identifier for species 3	CO
.	.	.	.
.	.	.	.
.	.	.	.
NSE4	C*12	Species identifier for species “NSE4”	SO2

* “NSE4” elements of CSLST4 array

[a] C*12 = Character*12

AREM.DAT - Header Record 3 - Molecular Weights

NO.*	TYPE[a]	DESCRIPTION	SAMPLE VALUES
1	R	Molecular weight for species 1	30.01 (NO)
2	R	Molecular weight for species 3	46.01 (NO2)
3	R	Molecular weight for species 3	28.01 (CO)
.	.	.	.
.	.	.	.
.	.	.	.
NSE4	R	Molecular weight for species “NSE4”	64.07 (SO2)

* “NSE4” elements of XMWEM1 array

[a] R = Real

AREM.DAT File - Data Records

The AREM.DAT file contains a set of "NSE4"+1 records for each time period (e.g., hour). The first data record of each set defines the time period over which the emissions data in the following records are valid. The next "NSE4" records each contain a species identifier and a two-dimensional gridded field of emissions.

Sample Fortran read statements for a set of data records are:

```
Loop over time periods (e.g., Hours)

READ(iunit)CID,XDATA,QEMIT

    Loop over species

    READ(iunit)CSPEC,QEMIT

    End loop over species

End loop over time periods
```

where the following declarations apply:

```
CHARACTER*12 CSPEC
REAL QEMIT(nx4,ny4)
```

AREM - Data Record Contents
(Record 1 of each set)

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	IBDAT	I	Beginning date for which data in this set is valid (YYJJJ, where YY=year, JJJ=Julian day)
2	IBTIM	I	Beginning time for which data in this set is valid (00-23) LST
3	IEDAT	I	Ending date for which data in this set is valid (YYJJJ, where YY=year, JJJ=Julian day)
4	IETIM	I	Ending time for which data in this set is valid (00-23) LST

Example:

Data Valid for 1 hour:

IBDAT=89183,IBTIM=00,IEDAT=89183,IETIM=00
IBDAT=89183,IBTIM=01,IEDAT=89183,IETIM=01
IBDAT=89183,IBTIM=02,IEDAT=89183,IETIM=02

Data Valid for 3 hour:

IBDAT=89183,IBTIM=00,IEDAT=89183,IETIM=02
IBDAT=89183,IBTIM=03,IEDAT=89183,IETIM=05
IBDAT=89183,IBTIM=06,IEDAT=89183,IETIM=08

[a]I = Integer

AREM - Data Record Contents
(Records 2, 3, . . . "NSE4"+1 each set)

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	CSPEC	C*12	Species identifier (up to 12 characters)
Next NSE4	QEMIT	R array	Area source emission rate (g/s) of species "CSPEC" for each grid column (QEMIT(nx4,ny4))

[a]C*12 = Character*12
R = Real

4.1.10 User-Specified Deposition Velocity Data File (VD.DAT)

The CALGRID model requires that the user specify the a method for determining dry deposition velocities for each species. In Input Group 3 of the control file, one of the following flags must be specified for each pollutant.

0 - no dry deposition (deposition velocities set to zero)
1 - resistance model used - pollutant deposited as a gas
2 - resistance model used - pollutant deposited as a particle
3 - user-specified deposition velocities used

Note that different methods can be used for different pollutants in the same CALGRID run.

If any species are flagged as using "user-specified" deposition velocities, CALGRID reads a formatted user-prepared data file with a 24-hour diurnal cycle of deposition velocities for each species flagged. The 24 values correspond to hours 01-24 (LST) of the simulated day. Twenty-four values must be entered for each flagged pollutant, even if the model run is for less than a full diurnal cycle. The units of the deposition velocities are m/s.

An example of a user-specified VD file is shown in Table 4.1.10. The VD.DAT file uses a control file format (see Section 4.1.1). All text outside the delimiters (!) is considered as user comment information and is echoed back but otherwise ignored by the input module. Each data line consists of a delimiter followed by the species name, 24 deposition velocities, and a terminating delimiter. The data may extend over more than one line. The line being continued must end with a comma. The control file format allows the use of repetition factors (e.g., 3 * 1.0 instead of 1.0, 1.0, 1.0). The order in which the species are entered in the file is not important. However, the file must end with an input group terminator (i.e., !END!).

The model checks that values have been entered for each species flagged as using user-specified deposition velocities. An error message is printed and execution of the run is terminated if any values are missing. The run will also terminate with an error message from the input routine if too many values are entered (i.e., more than 24 values for a particular pollutant). The species names must match those used in the chemical mechanism of the model.

Table 4.1-10
Sample user-specified deposition velocity file for two species

```
                DEPOSITION VELOCITY FILE (VD.DAT)
                ---------------------------------


     VD.DAT contains a 24-hour diurnal cycle of deposition
velocities for each species flagged as using user-specified values
in the control file (CALGRID.INP).

NOTE: Units are in m/s.
-----------------------


SPECIES
 NAME         Deposition Velocities (m/s)
-------       ---------------------------

! HNO3    =   5*1.5e-2, 4*1.7e-2, 3*1.8e-2, 3*1.9e-2, 3*1.7e-2, 6*1.5e-2 !
! SO2     =   5*0.8e-2,13*1.0e-2, 6*0.8e-2                               !

!END!
```

4.1.11 Chemical Mechanism Definition File (LMPBE221.MOD)

The CALGRID model uses procedures developed by Carter (1988) for the definition of the chemical mechanism. These procedures allow the chemical mechanism to be easily modified or exchanged without requiring extensive recoding.

The current chemical mechanism, identified as LMPBE221 contains 50 chemical species and 102 chemical reactions (see Section 2.7). Information regarding these species and reactions is contained in an input file to the model which, for the current chemical mechanism, is called LMBE221.MOD. The LMPBE22l.MOD file contains a detailed specification of the chemical mechanism, including the species names, specific reactions in the mechanism rate constants, photolysis data, and hydrocarbon lumping. It also contains the numbers and names of species which are treated as transported (advected) species or pseudo-steady-state species. These variables must be consistent with the control file varinbles in the CALGRID.INP file (see Section 4.1.1).

The chemical mechanism definition file is designed to be completely compatible with Carter's chemical mechanism generation software. LMPBE221.MOD is an output file from Carter's PREPGM program, which prepares the chemical mechanism. This input file will change only if the chemical mechanism is changed.

The format and contents of the chemical mechanism definition file are in Table 4.1.11. A detailed description of the chemical package is contained in Carter (1988). The LMPBE221.MOD file defining the current chemical mechanism is shown in Table 4.1.11-2. The species are listed in their compact notation in lines 5 through 46. The full list of reactions is contained in lines 197-333. Note that the line and column numbers are for reference purposes only and are not part of the actual input file.

TABLE 4.1.11

Organization of the `LMPBE22l.MOD` File used to Input the Chemical Mechanism into the CALGRID Model

Group	FORTRAN Format Code	No. Records[a]	Variables or Description[b]
1	(A8,' = MODEL FORMAT')	1	File format code. Should be 'MV:1/88A' for this format.
2	(A16, A65)	1	Date and time mechanism was prepared; mechanism label. (Both in TITLE.)
3	(12I6)	1	Number of species (NS); number of active species (NDY); number of constant species (NSC); number of buildup species (NB); number of dummy species (NDUM); number of reactions (NRXN); number of variable coef's (NCOEFV); index no. for first constant coefficient (NCOC1); index no. for last constant coefficient (NCOC2); number of photolysis sets (NHPOTK); number of kinetic parameters (LOCKBF); and number of wavelengths for data in photolysis sets (NPHOTK)
4	(2F10.2)		Default temperature (TEMPR) and reference temperature (TREF)

[a] If an expression is given which evaluates to a non-integer, it is rounded up to the next higher value. If expression evaluates to zero, there is no input for this group.

[b] See Table 11 for a description of the variables written into this file. Variables listed here which are not listed in Table 11 are local variables in WRITRX.

[c] "c" is total number of continuation lines for all reactions in the mechanism.

TABLE 4.1.11

Organization of the `LMPBE22l.MOD` File used to Input the Chemical Mechanism into the CALGRID Model

Group	FORTRAN Format Code	No. Records[a]	Variables or Description[b]
5	(A16, F7.2, F6.2, I3, 1PE11.3)	(NSC+ NB+ NDUM+ NDY)	Species name [NAME); default molecular weight (MWT); default number of carbons C-CNO); default number of nitrogens (NNO); and default initial concentrations for the constant, buildup, dummy, and active species, respectively.
6	(5A16)	(NS-NSC- NB-NDUM-NDY)/5	Species name (NAME) for the steady state species. No input if no steady state species in mechanism.
7	(4(A8, 1PE11.3, 1X))	NCOEFV/4	Name; value for all variable coef's. (COEFNM(I), COEF(I), I=l,NCOEFV)
8	(1P6E12.3)	(NCOC2-NCOC1+ 1)/6	Values for all constant coef's. (COEF(I), I=NCOCl, NCOC2).
9	One group of 4 records for each of the NPHOTK photolysis sets		

[a] If an expression is given which evaluates to a non-integer, it is rounded up to the next higher value. If expression evaluates to zero, there is no input for this group.

[b] See Table 11 for a description of the variables written into this file. Variables listed here which are not listed in Table 11 are local variables in WRITRX.

[c] "c" is total number of continuation lines for all reactions in the mechanism.

TABLE 4.1.11

Organization of the LMPBE22l.MOD File used to Input the Chemical Mechanism into the CALGRID Model

Group	FORTRAN Format Code	No. Records[a]	Variables or Description[b]
9a	(A8, I5, 7X, 1P6E10.3)	1	Photolysis set name; index for first reaction using this set; absorption coefficient x quantum yield values for the first 6 wavelengths. PHOTNM(I), IPHOTR(I), (AQ(I),I=1,6)
9b	(5E10.3)	3	Absorption coefficient x quantum yield values for rest of the NSOLWL wavelengths, where NSOLWL = 27. (AQ(I), I=7,27)
l0	(1P8E10.3)	LOCKBF/8	Kinetic parameter data. See Table 11. (KPBLJF(I), I=1, LOCKBF)
11	(16I5)	NRXN/16	Kinetic parameter index for each reaction. See Table 11. (LKBUF(I), I=1, NXRN)
12	(16I5)	NRXN/16	Kinetic parameter type for each reaction. See Table 11. (RXTYP(I), I=l,NRXN)
13	(10A8)	NRXN/8	Reaction labels. (RXNLBL(I), I=l,NRXN)
14	(L1, 1X, A78)	NRXNS+c[c]	Logical variable indicating whether there are additional input for this reaction (.TRUE. if none, .FALSE. if additional input for this reaction); part or all of reaction list.

[a] If an expression is given which evaluates to a non-integer, it is rounded up to the next higher value. If expression evaluates to zero, there is no input for this group.

[b] See Table 11 for a description of the variables written into this file. Variables listed here which are not listed in Table 11 are local variables in WRITRX.

[c] "c" is total number of continuation lines for all reactions in the mechanism.

Table 4.1.11-2

Listing of the chemical mechanism definition file (`LMPBE221.MOD`) used in the current version of the CALGRID model. The chemical mechanism is listed below in lines 171-291. Note that the line and column numbers are for reference purposes only and are not part of the actual input file.

```
Line Column   1         2         3         4         5         6         7         8
 No. 12345678901234567890123456789012345678901234567890123456789012345678901234567890
   1 MV:1/88A = MODEL FORMAT
   2 08-MAY-88 17:20 MODEL=carbon4.   LUMP LEVEL 2;  4 ALKAROS, 2 ALKENES.  NO XOOH
   3     41    33     4     0     0    84   140   421   460    11   165    27
   4     298.00    298.00
   5 O2                32.00  0.00  0  2.090E+05
   6 M                 28.85  0.00  0  1.000E+06
   7 HV                 0.00  0.00  0  1.000E+00
   8 H2O               18.02  0.00  0  2.000E+04
   9 NO                30.01  0.00  1  0.000E-01
  10 NO2               46.01  0.00  1  0.000E-01
  11 O3                48.00  0.00  0  0.000E-01
  12 HONO              47.02  0.00  1  0.000E-01
  13 HNO3              63.02  0.00  1  0.000E-01
  14 PNA                0.00  2.00  1  0.000E-01
  15 N2O5             108.02  0.00  2  0.000E-01
  16 NO3               62.01  0.00  1  0.000E-01
  17 HO2.              33.01  0.00  0  0.000E-01
  18 CO                28.01  1.00  0  0.000E-01
  19 FORM              30.03  1.00  0  0.000E-01
  20 ALD2              44.05  2.00  0  0.000E-01
  21 PAN              121.05  2.00  1  0.000E-01
  22 XO2                0.00  0.00  0  0.000E-01
  23 C2O3              72.00  2.00  0  0.000E-01
  24 CRO                0.00  0.00  0  0.000E-01
  25 MGLY              72.07  3.00  0  0.000E-01
  26 PAR               14.03  1.00  0  0.000E-01
  27 ETH               28.05  2.00  0  0.000E-01
  28 OLE               28.06  2.00  0  0.000E-01
  29 TOL               92.13  7.00  0  0.000E-01
  30 XYL              106.16  8.00  0  0.000E-01
  31 OPEN               0.00  5.00  0  0.000E-01
  32 CRES             108.14  7.00  0  0.000E-01
  33 TO2                0.00  0.00  0  0.000E-01
  34 ROR                0.00  0.00  0  0.000E-01
  35 H2O2              34.00  0.00  0  0.000E-01
  36 ISOP              68.11  6.00  0  0.000E-01
  37 MEOH              32.04  1.00  0  0.000E-01
  38 ETOH              46.07  2.00  0  0.000E-01
  39 SO2               64.07  0.00  0  0.000E-01
  40 SO3               80.07  0.00  0  0.000E-01
  41 UNR               16.01  1.00  0  0.000E-01
  42 OH              O               O1D             XO2N
  43 LITTLE    1.000E-30 QY.MEK    1.000E-01 A1RR      0.000E-01 A1NR      0.000E-01
  44 A1RXN     0.000E-01 A1RH      0.000E-01 A1R2      0.000E-01 A1RO2     0.000E-01
  45 A1A1X     0.000E-01 A1A2X     0.000E-01 A1K4X     0.000E-01 A1CO      0.000E-01
  46 A1C2      0.000E-01 A1CRES    0.000E-01 A1MG      0.000E-01 A1U2      0.000E-01
```

```
 47 A1XC      0.000E-01 A1NC      0.000E-01 A1XN      0.000E-01 A1NP      0.000E-01
 48 A1A1      0.000E-01 A1A2      0.000E-01 A1A3      0.000E-01 A1K3      0.000E-01
 49 A1K4      0.000E-01 A1PH      0.000E-01 A1CR      0.000E-01 A1BZ      0.000E-01
 50 A1GL      0.000E-01 A2RR      0.000E-01 A2NR      0.000E-01 A2RXN     0.000E-01
 51 A2RH      0.000E-01 A2R2      0.000E-01 A2RO2     0.000E-01 A2A1X     0.000E-01
 52 A2A2X     0.000E-01 A2K4X     0.000E-01 A2CO      0.000E-01 A2C2      0.000E-01
 53 A2CRES    0.000E-01 A2MG      0.000E-01 A2U2      0.000E-01 A2XC      0.000E-01
 54 A2NC      0.000E-01 A2XN      0.000E-01 A2NP      0.000E-01 A2A1      0.000E-01
 55 A2A2      0.000E-01 A2A3      0.000E-01 A2K3      0.000E-01 A2K4      0.000E-01
 56 A2PH      0.000E-01 A2CR      0.000E-01 A2BZ      0.000E-01 A2GL      0.000E-01
 57 A3RR      0.000E-01 A3NR      0.000E-01 A3RXN     0.000E-01 A3RH      0.000E-01
 58 A3R2      0.000E-01 A3RO2     0.000E-01 A3A1X     0.000E-01 A3A2X     0.000E-01
 59 A3K4X     0.000E-01 A3CO      0.000E-01 A3C2      0.000E-01 A3CRES    0.000E-01
 60 A3MG      0.000E-01 A3U2      0.000E-01 A3XC      0.000E-01 A3NC      0.000E-01
 61 A3XN      0.000E-01 A3NP      0.000E-01 A3A1      0.000E-01 A3A2      0.000E-01
 62 A3A3      0.000E-01 A3K3      0.000E-01 A3K4      0.000E-01 A3PH      0.000E-01
 63 A3CR      0.000E-01 A3BZ      0.000E-01 A3GL      0.000E-01 A4RR      0.000E-01
 64 A4NR      0.000E-01 A4RXN     0.000E-01 A4RH      0.000E-01 A4R2      0.000E-01
 65 A4RO2     0.000E-01 A4A1X     0.000E-01 A4A2X     0.000E-01 A4K4X     0.000E-01
 66 A4CO      0.000E-01 A4C2      0.000E-01 A4CRES    0.000E-01 A4MG      0.000E-01
 67 A4U2      0.000E-01 A4XC      0.000E-01 A4NC      0.000E-01 A4XN      0.000E-01
 68 A4NP      0.000E-01 A4A1      0.000E-01 A4A2      0.000E-01 A4A3      0.000E-01
 69 A4K3      0.000E-01 A4K4      0.000E-01 A4PH      0.000E-01 A4CR      0.000E-01
 70 A4BZ      0.000E-01 A4GL      0.000E-01 O1NC      0.000E-01 O1P1      0.000E-01
 71 O1P2      0.000E-01 O1P3      0.000E-01 O1P4      0.000E-01 O1P5      0.000E-01
 72 O1PN      0.000E-01 O1GA      0.000E-01 O1P1R     0.000E-01 O1P23R    0.000E-01
 73 O1P45R    0.000E-01 O1PR      0.000E-01 O1OHXC    0.000E-01 O1O3A1    0.000E-01
 74 O1O3A2    0.000E-01 O1O3K4    0.000E-01 O1O3MG    0.000E-01 O1O3CO    0.000E-01
 75 O1O3SB    0.000E-01 O1O3RH    0.000E-01 O1O3OH    0.000E-01 O1O3RR    0.000E-01
 76 O1O3R2    0.000E-01 O1O3RO2   0.000E-01 O1O3PS    0.000E-01 O1O3XC    0.000E-01
 77 O1OAXC    0.000E-01 O1P23     0.000E-01 O1P45     0.000E-01 O1N3XC    0.000E-01
 78    2.000E+00   5.000E-01   1.500E+00   1.550E-01   2.055E+00   1.600E-01
 79    1.100E-01   1.390E+00   1.070E-01   1.500E-01   8.500E-01   2.000E-01
 80    8.500E-02   5.805E+00   3.500E+00   2.200E-01   1.560E+00   3.700E-01
 81    4.400E-01   5.600E-01   1.200E-01   4.000E-01   7.500E-01   3.000E-01
 82    3.300E-01   5.000E+00   4.000E+00   7.000E+00   3.000E+00   1.000E+00
 83    5.000E-02   2.500E-01   1.400E-01   2.100E-01   1.000E-01   7.500E-02
 84    1.850E-01   6.000E-02   1.050E-01   1.350E-01
 85 NO2         1        9.525E-20 1.149E-19 1.616E-19 1.707E-19 2.178E-19 2.446E-19
 86  2.856E-19 3.286E-19 3.678E-19 3.842E-19 3.845E-19 4.206E-19 4.515E-19 5.387E-19
 87  4.801E-19 4.596E-19 8.660E-20 1.154E-20 0.000E-01 0.000E-01 0.000E-01 0.000E-01
 88  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
 89 O3O3P       8        0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
 90  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
 91  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
 92  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
 93 O3O1D       9        6.903E-19 3.528E-19 1.786E-19 5.768E-20 6.264E-21 0.000E-01
 94  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
 95  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
 96  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
 97 NO3        14        0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
 98  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
 99  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
100  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
101 HONO       23        9.300E-21 7.100E-21 5.400E-21 4.200E-21 3.200E-21 2.500E-21
102  1.900E-21 1.400E-21 1.100E-21 8.000E-22 6.000E-22 5.000E-22 0.000E-01 0.000E-01
```

```
103  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
104  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
105 H2O2       34        0.000E-01 0.000E-01 0.000E-01 0.000E-01 4.200E-21 2.100E-20
106  4.040E-20 7.290E-20 6.450E-20 1.050E-19 8.540E-20 6.830E-20 6.830E-20 1.190E-19
107  7.780E-20 1.200E-20 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
108  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
109 FORMRAD    38        2.472E-20 5.760E-21 3.903E-20 7.828E-21 2.016E-20 1.043E-20
110  1.073E-20 6.368E-21 2.600E-23 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
111  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
112  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
113 FORMSTAB   39        7.383E-21 1.440E-21 1.037E-20 2.472E-21 8.640E-21 6.669E-21
114  1.117E-20 1.156E-20 1.240E-22 6.420E-21 6.240E-22 1.170E-22 0.000E-01 0.000E-01
115  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
116  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
117 ALD2       45        2.160E-20 1.849E-20 1.258E-20 7.425E-21 3.570E-21 1.800E-21
118  4.400E-22 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
119  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
120  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
121 OPEN       69        0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
122  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
123  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
124  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
125 MGLY       74        0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
126  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
127  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
128  0.000E-01 0.000E-01 0.000E-01 0.000E-01 0.000E-01
129  8.384E+04 1.175E+03 0.000E+00 2.643E+03-1.370E+03 0.000E+00 1.375E+04 2.303E+02
130  6.870E+02 0.000E+00 3.233E+02 6.020E+02 0.000E+00 1.760E+02-2.450E+03 0.000E+00
131  5.300E-02 1.147E+05 3.900E+02 0.000E+00 3.260E+00 2.344E+03-9.400E+02 0.000E+00
132  2.100E+01-5.800E+02 0.000E+00 3.390E+01 1.909E+04 2.500E+02 0.000E+00 3.660E+01
133 -1.230E+03 0.000E+00 7.849E+02 2.560E+02 0.000E+00 1.900E-06 2.110E+16-1.090E+04
134  0.000E+00 2.600E-05 5.300E+02 0.000E+00 1.600E-11 6.554E+02 8.060E+02 0.000E+00
135  1.975E-01 9.770E+03 1.500E-05 1.537E+03 7.130E+02 0.000E+00 7.600E+00 1.000E+03
136  0.000E+00 5.482E+03 2.400E+02 0.000E+00 0.000e+00 0.000e+02 0.000E+00 0.000e+00
137  0.000e+04 0.000E+00 0.000e+00 0.000e+02 0.000E+00 8.739E+01 1.150E+03 0.000E+00
138  7.690E-10 5.800E+03 0.000E+00 2.550E-01 4.720E+03-1.870E+02 0.000E+00 3.220E+02
139  1.500E+04 4.302E+04-1.550E+03 0.000E+00 9.300E-01 1.739E+04-9.860E+02 0.000E+00
140  1.037E+04 2.500E+02 0.000E+00 3.700E+00 5.170e+04-1.800E+02 0.000E+00 3.830E+03
141  3.800E+02 0.000E+00 1.200E+18-1.350E+04 0.000E+00 3.700E+03 9.600E+03 6.521E+03
142 -1.710E+03 0.000E+00 1.203E+03 6.250E+16-8.000E+03 0.000E+00 9.545E+04 2.200E+04
143  1.756E+04-3.240E+02 0.000E+00 7.740E+03 5.040E+02 0.000E+00 2.104E+01-2.105E+03
144  0.000E+00 1.135E+01 1.540E+04-7.920E+02 0.000E+00 3.000E+03 4.110E+02 0.000E+00
145  1.856E+01-2.633E+03 0.000E+00 3.106E+03 3.220E+02 0.000E+00 1.200E+04 2.500E+02
146  6.100E+04 3.250E+04 2.000E+04 9.040E+00 4.400E+04 8.030E-02-5.000E+02 0.000E+00
147  2.453E+04 1.160E+02 0.000E+00 2.600E+04 9.640E+00 2.700E+04 1.520E+05 1.800E-02
148  4.700E+02 1.200E+04 2.550E+01 1.300E+03 0.000E-01 1.000E+03 1.113E+03 1.600E+02
149  0.000E+00 1.600E+03 2.380E+03 1.760E+02 0.000E+00
150     1    1    4    7    8   11   14   17    2   18   21   22   25   28   29   32
151    35   38   39   42   45   46   49   50   51   52   55   58   61   64   67   70
152    73   76   77   80   81    3    4   82   85   86   89   92    5   93   96   99
153   102  103  104  107  108  111  112  113  116  119  122  123  126  129  132  135
154   136  137  138  139  140  141  142  145  148  149  150  151  152  153  154  155
155   158  159  162  163
156     7    4    4    3    4    4    4    1    7    4    3    4    4    1    4    4
157     4    3    4    4    3    4    1    3    3    4    4    4    4    4    4    4
158     4   39    4    3    3    7    7    4    3    4    4    3    7    4    4    4
```

```
159     3    3    4    3    4    3    3    4    4    4    3    4    4    4    4    3
160     3    3    3    3   38    3    4    4    3   38    3    3    3    3    3    4
161     3    4    3    4
162     1       2       3A      3B      4       5       6       7       8       9
163     10      11      12A     12B     13A     13B     14      15      16      17
164     18      19      21      22      23      24      25      27      28      29A
165     29B     29C     29D     30A     30B     30C     30A     33      B1      B5
166     B8      B2      B4      B6      B9      B10     C18     B11     B12     B13
167     B14     B19     B20     B21     B22     B15     B16     B17     B18     G2
168     G3      G4      G5      C1      C2      C3      C4      C4A     C4B     C9
169     C10     C11A    C12     C44     C57     C95     C68A    C68B    C69     C70
170     SR1     SO2     MEOH    ETOH
171 T NO2 = 1.0 NO + 1.0 O
172 T O  = 1.0 O3
173 T NO + O3 = 1.0 NO2
174 T O + NO2 = 1.0 NO
175 T O + NO2 = 1.0 NO3
176 T O + NO = 1.0 NO2
177 T O3 + NO2 = 1.0 NO3
178 T O3 = 1.0 O
179 T O3 = 1.0 O1D
180 T O1D = 1.0 O
181 T O1D + H2O = 2.0 OH
182 T O3 + OH = 1.0 HO2
183 T O3 + HO2 = 1.0 OH
184 F NO3 = 0.89 NO2 + 0.89 O + &
185 T 0.11 NO
186 T NO3 + NO = 2.0 NO2
187 T NO3 + NO2 = 1.0 NO + 1.0 NO2
188 T NO3 + NO2 = 1.0 N2O5
189 T N2O5 + H2O = 2.0 HNO3
190 T N2O5 = 1.0 NO3 + 1.0 NO2
191 T NO + NO = 2.0 NO2
192 T NO + NO2 + H2O = 2.0 HONO
193 T NO + OH = 1.0 HONO
194 T HONO = 1.0 OH + 1.0 NO
195 T OH + HONO = 1.0 NO2
196 F HONO + HONO = 1.0 NO + &
197 T 1.0 NO2
198 T NO2 + OH = 1.0 HNO3
199 T OH + HNO3 = 1.0 NO3
200 T HO2 + NO = 1.0 OH + 1.0 NO2
201 T HO2 + NO2 = 1.0 PNA
202 T PNA = 1.0 HO2 + 1.0 NO2
203 T PNA + OH = 1.0 NO2
204 T HO2 + HO2 = 1.0 H2O2
205 T HO2 + HO2 + H2O = 1.0 H2O2
206 T OH  + H2O2 = 1.0 HO2
207 T OH  + CO = 1.0 HO2
208 T FORM + OH = 1.0 HO2  + 1.0 CO
209 T FORM = 2.0 HO2 + 1.0 CO
210 T FORM = 1.0 CO
211 T H2O2 = 2.0 OH
212 F FORM + O = 1.0 OH + &
213 T 1.0 HO2 + 1.0 CO
214 F FORM + NO3 = 1.0 HNO3 + &
```

```
215 T 1.0 HO2 + 1.0 CO
216 T ALD2 + O = 1.0 C2O3 + 1.0 OH
217 T ALD2 + OH = 1.0 C2O3
218 F ALD2 + NO3 = 1.0 C2O3 + &
219 T 1.0 HNO3
220 F ALD2 = 1.0 FORM + 2.0 HO2 + &
221 T 1.0 CO + 1.0 XO2
222 F C2O3 + NO = 1.0 FORM + &
223 T 1.0 NO2 + 1.0 HO2 + 1.0 XO2
224 T C2O3 + NO2 = 1.0 PAN
225 T PAN = 1.0 C2O3 + 1.0 NO2
226 F C2O3 + C2O3 = 2.0 XO2 + &
227 T 2.0 FORM + 2.0 HO2
228 F C2O3 + HO2 = 0.79 FORM + &
229 T 0.79 XO2 + 0.79 HO2 + 0.79 OH
230 F OH = 1.00 XO2  + 1.0 FORM + &
231 T 1.0 HO2
232 F PAR + OH = 0.87 XO2 + &
233 T 0.13 XO2N + 0.11 HO2
234 F ROR = 1.10 ALD2 + 0.96  XO2 + &
235 F 0.94 HO2 + 0.04 XO2N + &
236 T 0.02  ROR - 2.10 PAR
237 T ROR = 1.0 HO2
238 T ROR + NO2 =
239 F O + OLE = 0.63 ALD2 + 0.38 HO2 + &
240 F 0.28 XO2 + 0.30 CO + 0.20 FORM + &
241 T 0.02 XO2N + 0.22 PAR + 0.20 OH
242 F OH + OLE = 1.0 FORM + 1.0 ALD2 + &
243 T 1.0 XO2 + 1.0 HO2 - 1.0 PAR
244 F O3 + OLE = 0.5 ALD2 + 0.74 FORM + &
245 F 0.22 XO2 + 0.1 OH + 0.33 CO &
246 T + 0.44 HO2 - 1.0 PAR
247 F NO3 + OLE = 0.91 XO2 + 1.0 FORM + &
248 F 0.09 XO2N + 1.0 ALD2 + &
249 T 1.0 NO2 - 1.0 PAR
250 F O + ETH = 1.0 FORM + 1.7 HO2 + &
251 T 1.0 CO + 0.7 XO2 + 0.3 OH
252 F OH + ETH = 1.0 XO2 + 1.56 FORM + &
253 T 0.22 ALD2 + 1.0 HO2
254 F O3 + ETH = 1.0 FORM + 0.42 CO + &
255 T 0.12 HO2
256 F TOL + OH = 0.44 HO2 + 0.08 XO2 + &
257 T 0.36 CRES + 0.56 TO2
258 F TO2 + NO = 0.90 NO2 + 0.90 HO2 + &
259 T 0.90 OPEN
260 T TO2 = 1.0 CRES + 1.0 HO2
261 F OH + CRES = 0.4 CRO + 0.6 XO2 + &
262 T 0.6 HO2 + 0.3 OPEN
263 T CRES + NO3 = 1.0 CRO + 1.0 HNO3
264 T CRO + NO2 =
265 T OPEN - 1.0 C2O3 + 1.0 HO2 + 1.0 CO
266 F OPEN + OH = 1.0 XO2 + 2.0 CO + &
267 T 2.0 HO2 + 1.0 C2O3 + 1.0 FORM
268 F OPEN + O3 = 0.03 ALD2 + 0.62 C2O3 + &
269 F 0.70 FORM + 0.03 XO2 + 0.69 CO + &
270 T 0.08 OH + 0.76 HO2 + 0.20 MGLY
```

```
271 F XYL + OH = 0.70 HO2 + 0.50 XO2 + &
272 F 0.20 CRES + 0.80 MGLY + 0.30 TO2 + &
273 T 1.10 PAR
274 T MGLY + OH = 1.0 C2O3 + 1.0 XO2
275 T MGLY = 1.0 C2O3 + 1.0 HO2 + 1.0 CO
276 F ISOP + O = 0.6 HO2 + 0.8 ALD2 + &
277 F 0.55 OLE + 0.5 XO2 + &
278 T 0.5 CO + 0.45 ETH + 0.90 PAR
279 F ISOP + OH = 1.0 XO2 + 1.00 FORM + &
280 F 0.67 HO2 + 0.4 MGLY + 0.20 C2O3 + &
281 T 1.00 ETH + 0.2 ALD2 + 0.13 XO2N
282 F ISOP + O3 = 1.0 FORM + 0.40 ALD2 + &
283 F 0.55 ETH + 0.2 MGLY + 0.44 HO2 + &
284 T 0.06 CO + 0.10 PAR + 0.1 OH
285 T ISOP + NO3 = 1.0 XO2N
286 T XO2 + NO = 1.0 NO2
287 T XO2 + XO2 =
288 T XO2N + NO =
289 T SO2N + OH = SO3
290 T MEOH + OH = FORM + HO2
291 T ETOH + OH =
```

4.1.12 Emission-Specific Chemical Data File (CALBE221.RXP)

The CALGRID model makes use of the outputs of the emission preparation system developed by Carter (1988). This system is designed to process emissions data to be consistent with the specific chemical mechanism used in CALGRID (i.e., classifying the hydrocarbon emissions according to the lumping scheme used), and adjusts emissions-specific parameters of the chemical mechanism.

for the definition of the chemical mechanism. These procedures allow the chemical mechanism to be easily modified or exchanged without requiring extensive recoding.

The current chemical mechanism in CALGRID CMPBE221, uses an emission-specific file called CALBE221.RXP. This file is an output of the PREPEMIT program which is part of Carter's system. The data in CALBE221.RXP is read only once in the setup phase of CALGRID. It is necessary to rerun the PREPEMIT program any time there is a change in the "typical" emission profile, the lumping approach used in the chemical mechanism, or any kinetic or mechanistic parameters for emitted organic species (Carter, 1988). The user should refer to Carter's documentation for details on executing the PREPEMIT program and the other components of the emissions processing system.

Table 4.1.12 contains a sample emissions specific chemical data file (CALBE221.RXP) which was used in the preliminary testing of the CALGRID model.

Table 4.1.12

A sample emissions-specific data file (CALBE221.RXP) used the preliminary testing of the CALGRID model. This file must be modified to be consistent with the particular emissions inventory and chemical mechanism being used in the CALGRID modeling. It is an output of the PREPEMIT emissions processing program (Carter, 1988).

```
! Emissions input file =   TS082787.EMI
! Lumping control file =   COND2243
! SAROAD assignment file = SAROAD2.PRM,  format = ARB
! Lumping temperature    = 300.00
!
! Normalized to 1 mole NMHC.  Factor = 9.0544E-06
!
! Total wt. (g)           =  23.698
! Wt. percent of unknowns =   0.056
! Total number of moles   =  0.7592
! Total number of moles C =  1.5181
! No. model species used  =  174
! Normalization checked OK.
!
!
!    GROUP = ALK1,  PARAMETER AVERAGES WEIGHED BY ESTIMATED AMOUNT REACTED,
!                   BASED ON INTEGRATED OH =  8.20E-05 PPM-MIN.
!                   FRACTION REACTING (MOLAR) = 0.5693
!
!                 MOLES       MOLES C    C/MOLE    M.W.
!      TOTAL    1.0736E-01  3.5823E-01    3.337    55.90
!     REACTING  6.1124E-02  2.7269E-01    4.461    69.17
!      LOST     4.6234E-02  8.5545E-02    1.850    38.36
!
K(A1OH)   5.4831E+03
A1NC      4.4612E+00
A1NR      7.3710E-02
A1XN      4.2156E-03
A1RR      7.7452E-01
A1R2      4.5040E-01
A1A1      4.3650E-02
A1A2      2.4137E-01
A1K3      3.4833E-01
A1A3      1.7392E-01
A1K4      4.3142E-01
A1CO      1.0687E-02
A1XC      6.9047E-02
A1RH      1.4755E-01
!
!    GROUP = ALK2,  PARAMETER AVERAGES WEIGHED BY AMOUNT PRESENT
!                   (SUITABLE FOR FASTER REACTING SPECIES).
!
!                 MOLES       MOLES C    C/MOLE    M.W.
!      TOTAL    2.5460E-02  1.9122E-01    7.511   110.14
!
K(A2OH)   1.5488E+04
```

```
A2NC      7.5107E+00
A2NR      2.1217E-01
A2XN      1.2462E-03
A2RR      7.1725E-01
A2R2      7.4196E-01
A2A1      5.8713E-02
A2A2      8.3578E-02
A2K3      3.5594E-03
A2A3      3.2982E-01
A2K4      9.9049E-01
A2CO      1.4411E-02
A2C2      1.7955E-02
A2XC      1.1432E+00
A2RH      6.9209E-02
!
!    GROUP = ARO1,  PARAMETER AVERAGES WEIGHED BY ESTIMATED AMOUNT REACTED,
!                   BASED ON INTEGRATED OH =  8.20E-05 PPM-MIN.
!                   FRACTION REACTING (MOLAR) = 0.8948
!
!                 MOLES       MOLES C    C/MOLE    M.W.
!      TOTAL    1.8690E-02  1.3056E-01    6.985    91.94
!     REACTING  1.6724E-02  1.1917E-01    7.126    93.91
!      LOST     1.9663E-03  1.1386E-02    5.791    75.24
!
!                   AVG KOH = 8.5066E+03, BUT DEFAULT OF 8.6690E+03 USED
!
K(B1OH)   8.6690E+03
B1NC      7.1258E+00
B1RR      7.4122E-01
B1RH      2.5878E-01
B1CR      2.5878E-01
B1MG      1.2435E-01
B1U2      3.8514E-01
!
!    GROUP = ARO2,  PARAMETER AVERAGES WEIGHED BY AMOUNT PRESENT
!                   (SUITABLE FOR FASTER REACTING SPECIES).
!
!                 MOLES       MOLES C    C/MOLE    M.W.
!      TOTAL    1.0248E-02  8.7795E-02    8.567   114.05
!
K(B2OH)   4.4017E+04
B2NC      8.5672E+00
B2RR      8.1883E-01
B2RH      1.7826E-01
B2NP      2.9108E-03
B2CR      1.7826E-01
B2MG      4.3984E-01
B2U2      6.1515E-01
!
!    GROUP = OLE1,  PARAMETER AVERAGES WEIGHED BY AMOUNT PRESENT
!                   (SUITABLE FOR FASTER REACTING SPECIES).
!
!                 MOLES       MOLES C    C/MOLE    M.W.
!      TOTAL    1.2787E-02  4.8523E-02    3.795    53.23
!
K(O1OH)   4.4214E+04
```

```
O1NC      3.7946E+00
O1P1      1.0000E+00
O1P2      6.0968E-01
O1P3      3.1379E-01
O1P4      7.6535E-02
O1PN      3.8644E-02
K(O1O3)   1.7375E-02
K(O1N3)   5.0156E+01
K(O1OA)   7.2417E+03
!
!    GROUP = OLE2,  PARAMETER AVERAGES WEIGHED BY AMOUNT PRESENT
!                   (SUITABLE FOR FASTER REACTING SPECIES).
!
!                 MOLES       MOLES C    C/MOLE    M.W.
!      TOTAL    4.9253E-03  2.3443E-02    4.760    66.37
!
K(O2OH)   9.4409E+04
O2NC      4.7597E+00
O2P1      1.8416E-01
O2P2      1.0266E+00
O2P3      6.4019E-01
O2P4      8.0096E-02
O2P5      3.2002E-02
O2PN      5.4508E-02
K(O2O3)   2.6362E-01
K(O2N3)   1.5569E+03
K(O2OA)   3.5102E+04
!
!    GROUP = OLE3,  PARAMETER AVERAGES WEIGHED BY AMOUNT PRESENT
!                   (SUITABLE FOR FASTER REACTING SPECIES).
!
!                 MOLES       MOLES C    C/MOLE    M.W.
!      TOTAL    7.6630E-03  5.0408E-02    6.578    89.62
!
K(O3OH)   1.5153E+05
O3NC      6.5781E+00
O3P1      7.2928E-01
O3P3      1.0000E+00
K(O3O3)   5.0543E-02
K(O3N3)   3.0863E+03
K(O3OA)   7.4775E+04
!
! SUMMARY OF EMITTED ROG SPECIES:
!
RHC(CH4 )  1.00    16.04
RHC(ETHE)  2.00    28.05
RHC(MEOH)  1.00    32.04
RHC(ETOH)  2.00    46.07
RHC(MTBE)  5.00    88.15
RHC(CO  )  1.00    28.01
RHC(HCHO)  1.00    30.03
RHC(CCHO)  2.00    44.05
RHC(RCHO)  3.00    58.08
RHC(MEK )  4.00    72.11
RHC(RNO3)  5.00   133.15
RHC(PAN )  2.00   121.05
```

```
RHC(PPN )  3.00   135.08
RHC(CRES)  7.00   108.14
RHC(MGLY)  3.00    72.07
RHC(AFG2)  3.00    72.07
RHC(ALK1)  4.46    69.17
RHC(ALK2)  7.51   110.14
RHC(ARO1)  7.13    93.91
RHC(ARO2)  8.57   114.05
RHC(OLE1)  3.79    53.23
RHC(OLE2)  4.76    66.37
RHC(OLE3)  6.58    89.62
!   NROG   1.00    20.56
!   LOST   1.00    17.58
```

4.2 Output Files

4.2.1 Concentration File (CONC.DAT)

The CONC.DAT file is an unformatted data file conatining gridded fields of one-hour average concentrations predicted by CALGRID. The creation and contents of the CONC.DAT file are controlled by user-specified inputs in Input Group 7 of the control file (see Section 4.1.1).

The control file variable ICON must be set equal to one in order to create the CONC.DAT file. The user also has control over the species and layers saved in the output file. Because of the multi-layer nature of the model and the large number of advected species (i.e, 36 in the current chemical mechanism), the user may not wish to save data for all species and all vertical layers. The control file output species table allows a selection to be made on a species by species basis of which vertical layers (if any) are to be stored in the CONC.DAT file.

The CONC.DAT file consists of three header records followed by a set of data records. The header records contain information describing the version of the model used in the run creating th file, horizontal and vertical grid data, a user-input title, and a list of the species/layer combinations stored in the output file.

The CONC.DAT file is designed to be compatible with the CALPUFF postprocessing programs. Several variables in the header records (such as the definitions of potentially different meteorological, computational, and sampling grids) are retained to maintain this compatibility even though they are not directly releveant to CALGRID.

Sample FORTRAN read statements for the header records are:

```
 READ(iunit)CMODEL,VER,LEVEL,IBYR,IBJUL,IBHR
1 IRLG,IAVG,NXM,NYM,DXKM,DYKM,NZ,IONE,NX,IONE,NY,
2 IONE,NX,IONE,NY,IONE,IZERO,IZERO,IZERO,IZERO,LSGRID,NSZOUT

 READ(iunit)TITLE

 READ(iunit)CSOUT
```

where the following declarations apply:

```
Character*80 TITLE(3)
Character*15 CSOUT(NSZOUT)
Character*12 CMODEL,VER,LEVEL
```

Unformatted CONC.DAT - Header Record 1 - General Data

NO.	VARIABLE	TYPE[a]	DESCRIPTION	SAMPLE VALUES
1	CMODEL	C*12	Model name	CALGRID
2	VER	C*12	Model version number	1.2
3	LEVEL	C*12	Model level number	890911
4	IBYR	I	Starting year of the run	80
5	IBJUL	I	Starting Julian day	183
6	IBHR	I	Starting hour (00-23)	8
7	IRLG	I	Length of run (hours)	5
8	IAVG	I	Averaging time (hours) of output concentrations (must be one hour for CALGRID output)	1
9	NXM	I	Number of grid points in meteorological grid (X direction)	20
10	NYM	I	Number of grid points in meteorological grid (Y direction)	20
11	DXKM	R	Grid spacing (km) in the X direction	5.
12	DYKM	R	Grid spacing (km) in the Y direction	5.
13	NZ	I	Number of vertical layers	10
14	IONE	I	Start of computational grid (X direction) (must be equal to one for CALGRID runs)	1
15	NX	I	End of computational grid (X direction) (must be equal to NX for CALGRID runs)	20
16	IONE	I	Start of sampling grid (Y direction) (must be equal to one for CALGRID runs)	1
17	NY	I	End of computational grid (Y direction) (must be equal to NX for CALGRID runs)	20
18	IONE	I	Start of sampling grid (X direction) (must be equal to one for CALGRID runs)	1
19	NX	I	End of sampling grid (X direction) (must be equal to NX for CALGRID runs)	20
20	IONE	I	Start of sampling grid (Y direction) (must be equal to one for CALGRID runs)	1

[a] C*12 = Character*12
I = Integer
R = Real
L = Logical

Unformatted CONC.DAT - Header Record 1 - General Data

NO.	VARIABLE	TYPE[a]	DESCRIPTION	SAMPLE VALUES
21	NY	I	End of sampling grid (Y direction) (must be equal to NX for CALGRID runs)	20
22	IONE	I	Sampling grid spacing factor (must be one for CALGRID runs)	1
23	IZERO	I	Unused by CALGRID	0
24	IZERO	I	Unused by CALGRID	0
25	IZERO	I	Unused by CALGRID	0
26	IZERO	I	Unused by CALGRID	0
27	LSGRID	L	Sampling grid flag (T = gridded receptors, F = no gridded receptors)	T
28	NSZOUT	I	Number of species-layer combinations stored in the output file	50

[a] C*12 = Character*12
I = Integer
R = Real
L = Logical

Unformatted CONC.DAT - Header Record 2 - Run Title

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	Title Array	C*80	User-specified run title (three lines of up to 70 characters/line)

Header Record 3 - List of Species-Layers in Output File

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	CSOUT Array	C*15	Species name (first 11 characters) and layer (last 3 characters) of concentrations stored in the output file

[a] C*80 = Character*80
C*15 = Character*15

CONC.DAT File - Data Records

The CONC.DAT data records consist of a set of "NSZOUT+1" records for each hour of the CALGRID run (NSZOUT is the number of species-layer combinations stored in the output file). The first record of each set contains the date and hour of the data in the records which follow it. The next "NSZOUT" records contain the predicted concentrations in ppm, for each species and layer flagged for output in the control file.

Sample FORTRAN read statements for the data records are:

```
LOOP OVER HOURS

READ(iunit)IBDAT, IBTIM, IEDAT, IETIM

    LOOP OVER SPECIES

        LOOP OVER LAYERS

        IF CURRENT SPECIES-LAYER COMBINATION S-
        TORED IN THE CONC.DAT FILE, THEN

        READ(iunit)CLABZ,XCOUT

        END LOOP OVER LAYERS

    END LOOP OVER SPECIES

END LOOP OVER HOURS
```

where the following declarations apply:

```
Character*15 CLABZ
Real XCOUT(nx,ny)
```

Unformatted CONC.DAT File - Data Records
(Record 1 of each set)

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	NYR	I	Year of concentration data (e.g., 80)
2	NJUL	I	Julian day of data
3	NHR	I	Hour (00-23) of data

(Records 2, 3, . . . , "NSOUT"+1 of each set)

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	CLABZ	C*15	Species name (first 12 characters) and layer (last 3 characters) of the concentrations in this record
Next NX*NY	XCOUT	R array	One-hour averaged concentrations (ppm) for each grid cell. The lateral boundary cells contain the boundary condition concentrations (ppm)

[a] I = Integer
C*15 = Character*15
R = Real

4.2.2 Dry Flux File (DFLX.DAT)

The DFLX.DAT file is an unformatted data file containing gridded fields of one-hour averaged dry deposition fluxes predicted by CALGRID. The creation and contents of the DFLX.DAT file are controlled by user-specified inputs in Input Group 7 of the control file (see Section 4.1.1).

The control file variable IDRY must be set equal to one in order to create the DFLX.DAT file. The species saved in the output file are also controlled by the user by setting flags in the output species table in Input Group 7 of the control file. The model checks that only advected species are flagged as being deposited, and only deposited species are flagged for output into the DFLX.DAT file. The effects of dry deposition on ambient concentrations can be evaluated without saving the dry fluxes in the output file if the actual values of the deposition fluxes are not of interest.

DFLX.DAT File - Header Records

The DFLX.DAT file consists of three header records followed by a set of data records. The header records contain information describing the version of the model used in the run creating the file, horizontal and vertical grid data, a user-input run title, and a list of the deposited species stored in the output file.

The DFLX.DAT file is designed to be compatible with the CALPUFF postprocessing programs. Several variables in the header records (such as the definition of potentially different meteorological, computational, and sampling grids) are retained to maintain this compatibility even though they are not directly relevant to CALGRID.

Sample FORTRAN read statements for the header records are:

```
 READ(iunit)CMODEL, VER, LEVEL, IBYR, IBJUL, IBHR, IRLG,
1 IAVG, NXM, NYM, DXKM, DYKM, NZ, lONE, NX, lONE, NY, IONE, NX,
2 IONE, NY, IONE, IZERO, IZERO, IZERO, IZERO, LSGRID, NDFOUT

 READ(iunit)TITLE

 READ(iunit)CDFOUT
```

where the following declarations apply:

```
Character*8O TITLE(3)
Character*15 CDFOUT(NDFOUT)
Character*12 CMODEL, VER, LEVEL
```

Unformatted DFLX.DAT - Header Record 1 - General Data

NO.	VARIABLE	TYPE[a]	DESCRIPTION	SAMPLE VALUES
1	CMODEL	C*12	Model name	CALGRID
2	VER	C*12	Model version number	1.2
3	LEVEL	C*12	Model level number	890911
4	IBYR	I	Starting year of the run	80
5	IBJUL	I	Starting Julian day	183
6	IBHR	I	Starting hour (00-23)	8
7	IRLG	I	Length of run (hours)	5
8	IAVG	I	Averaging time (hours) of output concentrations (must be one hour for CALGRID output)	1
9	NXM	I	Number of grid points in meteorological grid (X direction)	20
10	NYM	I	Number of grid points in meteorological grid (Y direction)	20
11	DXKM	R	Grid spacing (km) in the X direction	5.
12	DYKM	R	Grid spacing (km) in the Y direction	5.
13	NZ	I	Number of vertical layers	10
14	IONE	I	Start of computational grid (X direction) (must be equal to one for CALGRID runs)	1
15	NX	I	End of computational grid (X direction) (must be equal to NX for CALGRID runs)	20
16	IONE	I	Start of sampling grid (Y direction) (must be equal to one for CALGRID runs)	1
17	NY	I	End of computational grid (Y direction) (must be equal to NX for CALGRID runs)	20
18	IONE	I	Start of sampling grid (X direction) (must be equal to one for CALGRID runs)	1
19	NX	I	End of sampling grid (X direction) (must be equal to NX for CALGRID runs)	20
20	IONE	I	Start of sampling grid (Y direction) (must be equal to one for CALGRID runs)	1

[a] C*12 = Character*12
I = Integer
R = Real
L = Logical

Unformatted DFLX.DAT - Header Record 1 - General Data

NO.	VARIABLE	TYPE[a]	DESCRIPTION	SAMPLE VALUES
21	NY	I	End of sampling grid (Y direction) (must be equal to NX for CALGRID runs)	20
22	IONE	I	Sampling grid spacing factor (must be one for CALGRID runs)	1
23	IZERO	I	Unused by CALGRID	0
24	IZERO	I	Unused by CALGRID	0
25	IZERO	I	Unused by CALGRID	0
26	IZERO	I	Unused by CALGRID	0
27	LSGRID	L	Sampling grid flag (T = gridded receptors, F = no gridded receptors)	T
28	NDFOUT	I	Number of dry deposited species stored in the output file	50

[a] C*12 = Character*12
I = Integer
R = Real
L = Logical

Unformatted DFLX.DAT - Header Record 2 - Run Title

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	Title Array	C*80	User-specified run title (three lines of up to 70 characters/line)

Header Record 3 - List of Species-Layers in Output File

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	CDFOUT Array	C*15	Species name (first 11 characters) and layer (last 3 characters = '-DF') of this data stored in the output file

[a] C*80 = Character*80
C*15 = Character*15

DFLX.DAT - Data Records

The DFLX.DAT data records consist of a set of "INDFOUT"+1 records for each hour of the CALGRID runs (NDFOUT is the number of species flagged as being stored in the output file). The first record of each set contains the data and hour of the data in the records which follow it. The next "INDFOUT" records contain predicted one-hour averaged dry deposition fluxes in g/m^2/s for each relevant species.

Sample FORTRAN read statements for the data records are:

```
LOOP OVER HOURS

READ(iunit)IBDAT, IBTIM, IEDAT, IETIM

    LOOP OVER SPECIES

    IF CURRENT SPECIES STORED IN THE DFLX.DAT FILE, THEN

    READ(iunit)CLABDF,XDFOUT

    END LOOP OVER SPECIES

END LOOP OVER HOURS
```

where the following declarations apply:

```
Character*15 CLABDF
Real XDFOUT(nx, ny)
```

Unformatted DFLX.DAT File - Data Records
(Record 1 of each set)

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	NYR	I	Year of dry flux data (e.g., 80)
2	NJUL	I	Julian day of data
3	NHR	I	Hour (00-23) of data

(Records 2, 3, . . . , "NDFOUT"+1 of each set)

NO.	VARIABLE	TYPE[a]	DESCRIPTION
1	CLABDF	C*15	Species name (first 12 characters) and layer (last 3 characters = '-DF') of the data in this record
Next NX*NY	XDFOUT	R array	One-hour averaged dry deposition fluxes ($g/m^2/s$) for each grid cell. (Note: dry fluxes for boundary cells are not computed and therefore are zero).

[a] I = Integer
C*15 = Character*15
R = Real

5 REFERENCES

Briggs, G., 1973. Internal memo as reported by F.A. Gifford Jr. in Turbulent Diffusion-Typing Schemes: A Review. *Nuci. Saf.*, **17**, 68-86, 1976.

Briggs, G.A., 1975. Plume Rise Predictions. Lectures on Air Pollution and Environmental Impact Analyses, D.A. Haugen, Ed., American Meteorological Society, Boston, pp 59-111.

Carmichael, G.R., L.K. Peters, and T. Kitada, 1986. A Second Generation Model for Regional-Scale Transport/Chemistry/Deposition, *Atmos. Environ.*, **20**, 173-188.

Carter, W., 1988. Documentation for the SAPRC Atmospheric Photochemical Mechanism Preparation and Emissions Processing Programs for Implementation in Airshed Models, Draft report for California Air Resources Board.

Douglas, S. and R. Kessler, 1988. User's Guide to the Diagnostic Wind Model (Version 1.0). Systems Applications, Inc., San Rafael, CA.

Forester, C.K., 1977. Higher order monotonic convection difference schemes. *J. Camp. Phys.*, **23**: 1-22

Fowler, D. and M.H. Unsworth, 1979. Turbulent transfer of sulphur dioxide to a wheat crop. *Q.J. Roy. Meteor. Soc.*, **105**, 767-784.

Hesstvedt, E., O. Hov, and I.S.A. Isaksen, 1978. Quasi-steady-state approximations in air pollution modeling, *Comp. J. Chem. Kinetics*, Vol. X, 971-994.

Hicks, B.B., 1982. In: *Critical Assessment Document on Acid Deposition* (Chapter VII-Dry Deposition).. ATDL Contribution File No. 81/24. Atmospheric Turbulence and Diffusion Laboratory, NOM, Oak Ridge, TN.

Hosker, R.P., 1974. A Comparison of Estimation Procedures for Overwater Plume Dispersion. *Proceedings of the Symposium on Atmospheric Diffusion and Air Pollution*. American Meteorological Society, Boston, MA.

Hosker, R.P., Jr. and S.E. Lindberg, 1982. Review: Atmospheric Deposition and Plant Assimilation of gases and Particles. *Atmos. Environ.*, **16**, 889-910.

Kessler, R.C., 1989. User's Guide to the Systems Applications, Inc. Version of the Colorado State University Mesoscale Model (Version 2.0). Systems Applications, Inc., San Rafael, CA.

Lamb, R.G., 1984. A regional scale (1000 km) model of photochemical air pollution. Part 1 Theoretical formulation. EPA draft report.

Lurmann, F.W., A.C. Lloyd, and R. Atkinson, 1986. A Chemical Mechanism for use in Long-Range Transport/Acid Deposition Computer Modeling, JGR, 91, 10905.

Marchuk, G. I. 1975. *Methods of Numerical Mathematics*. New York: Springer-Verlag. 316 pp.

McRae, G., W. Goodin, and J. Seinfeld, 1982. Numerical Solution of the Atmospheric Diffusion Equation for Chemically Reacting Flows, *J. Comp. Phys.*, **95**, 1-42.

O'Dell, R.A., M. Taheri, and R.L. Kabel, 1977. A model for uptake of pollutants by vegetation. *JAPCA*, **27**, 1104-1109.

Peterson, J.T., 1976. Calculated Actinic Fluxes (290-700 nm) for Air Pollution Photochemistry Applications1 EPA-60014-76-025.

Pleim, J., A. Venkatram and R.J. Yamartino, 1984. *The Dry Deposition Model. Volume 4. ADOM/TADAP Model Development Program*. Ontario Ministry of the Environment, Rexdale, Ontario, Canada.

Reynolds, S.D., T.W. Tesche, and L.E. Reid, 1979. An Introduction to the SAI Airshed Model and its Usage. SAI Report EF78-53R4 - EF79-31.

Richards, J.M., 1971. A Simple Expression for the Saturation Vapor Pressure of Water in the Range - 50 to 140 C, *British J. Applied Physics D*, **4**, L25 - L18.

Scire, J.S., R.J. Yamartino, D.G. Strimaitis, S.R. Hanna, S. Douglas and R.C. Kessler, 1989. CALPUFF: A Non-Steady-State Air Quality Modeling System. Volume I: Model Formulation Document. California Air Resources Board, Sacramento, CA.

Scire, J.S., R.J. Yamartino, D.G. Strimaitis, S. Douglas and R. Kessler, 1989. CALPUFF: A Non-Steady-State Air Quality Modeling System. Volume II: User's Guide. California Air Resources Board, Sacramento, CA.

Shepherd, J.G., 1974. Measurements of the direct deposition of sulphur dioxide onto grass and water by the profile method. *Atmos. Environ.*, **8**, 69-74.

Slinn, S.A. and W.G.N. Slinn, 1980. Predictions for particle deposition on natural waters. *Atmos. Environ.*, **14**, 1013-1016.

Slinn, W.G.N., L. Hasse, B.B. Hicks, A.W. Hogan, D. Lal, P.S. Liss, K.O. Munnich, G.A. Sehmel, and 0. Vittori, 1978. Some aspects of the transfer of atmospheric trace constituents past the air-sea interface. *Atmos. Environ.*, **12**, 2055-2087.

Smagorinsky, J., 1963. General circulation experiments with the primitive equations: 1. The basic experiment. *Mon. Wea. Rev.* **91**: 99-164.

Voldner, E.C., L.A. Barrie, and A. Sirois, 1986. A literature review of dry deposition of oxides of sulphur and nitrogen with emphasis on longrange transport modeling in North America. *Atmos. Environ.*, **20**, 2101-2123.

Wesely, M.L. and B.B. Hicks, 1977. Some factors that affect the deposition rates of sulfur dioxide and Similar gases on Vegetation. *J. Air Poll. Control Assoc.*, **27**, 1110-1116.

Yamartino, R.J., J.S. Scire, S.R. Hanna, G.R. Carmichael and Y.S. Chang, 1989. CAL-GRID: A Mesoscale Photochernical Grid Model. Volume I: Model Formulation Document. California Air Resources Board, Sacramento, CA.

Young, T.R. and J.P. Boris, 1977. A Numerical Technique for Solving Stiff Ordinary Differential Equations Associated with the Chemical Kinetics of Reaction Flow Problems, *J. Phys. Chem.*, **82**, 2424.